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A Message from the Office of Science

At the Department of Energy, we understand that solving the Nation's substantial energy, environment, and national security problems requires the concerted efforts of many scientists. Training the next generation of scientists is one of our priorities.

The research studies featured in this volume of the *Journal of Undergraduate Research* detail a mentoring process that equips tomorrow's scientists with the skills and experience they need to meet our nation's challenges. Through an internship process, undergraduates from many different backgrounds begin their careers under the tutelage of accomplished scientists at our National Laboratories. Their work – a selection of which is showcased here – may contain the seeds of ideas that will change our world.

We believe today's investment in our scientists of the future will spark innovation that will maintain our role as world leader in science. I commend these young scientists for their achievements. I thank them and their mentors for their dedication to the scientific process and wish them continued success in their scientific pursuits.

A handwritten signature in dark ink, appearing to read "Patricia M. Dehmer".

Patricia M. Dehmer
Acting Director



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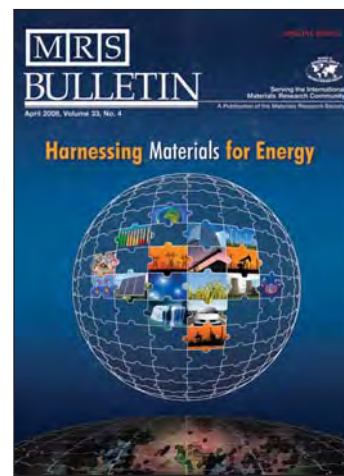
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A TIPPING POINT FOR SCIENCE

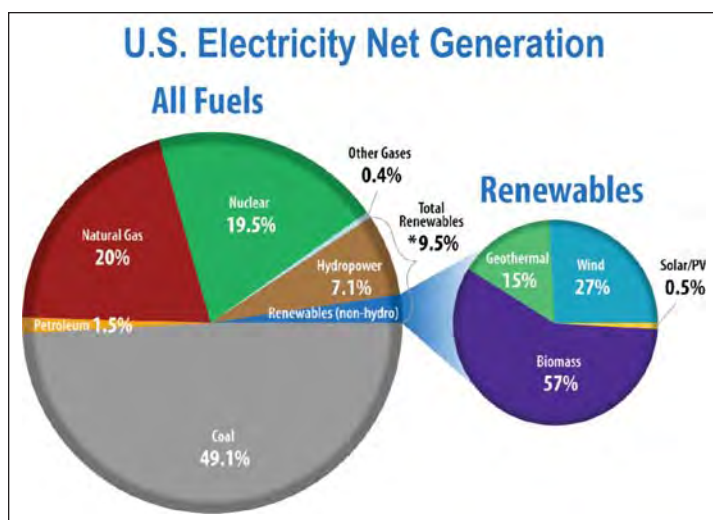
Undergraduates engaged in research at the National Laboratories often feel that their efforts to advance scientific knowledge are insignificant, or, at best, incremental contributions. Nothing could be further from the truth. Society (and perhaps even the planet) is at a crisis point and needs new perspectives and passions to create critically needed change. In *The Tipping Point*, Malcolm Gladwell contends that even seemingly small things can make a big difference. It is Gladwell's thesis that technological ideas and societal behaviors, including themes and even products, behave like outbreaks of infectious disease; they are in fact "social epidemics." The tipping points that he refers to are the levels at which the momentum for change becomes unstoppable. Such a tipping point may be triggered by increased societal or technological changes, even seemingly insignificant changes such as those initiated by undergraduate interns. One example of such an innovation is the Lithium (Li) battery. Small portable electronic devices like iPods and digital cameras, ubiquitous in today's world, would not have been possible without the advent of Li batteries. In this case, the Li battery triggered a tipping point, after a great deal of what must have seemed like insignificant, incremental research.

Currently, we may be at a nexus of tipping points, which creates an extraordinary opportunity for coupled societal and technological change that is unprecedented in modern times. The recent economic downturn, political unrest around the world, worries about global warming and an increasing belief that "business as usual" may not work has created a set of concurrent tipping points that could lead to the early adoption of new technologies and to sweeping changes in how we live. Although many of these ideas supporting sustainability have been advocated for by a small percentage of the population for a long time, and some have even been generally acknowledged as good ideas, they have never reached the critical mass that leads to widespread adoption. Historically, the ability of technology to drive societal change has been limited, and often ideas that seem to make "common sense" meet barriers that prevent their adoption. A unique opportunity exists today when those barriers have been lowered and profound change can occur. In fact, the current generation of students in our educational system will be the ultimate engine of this change and the ones that will actually implement it.

The Materials Research Society (MRS) recently published a special expanded bulletin, "Harnessing Materials for Energy," Volume 33, No. 4, on the materials challenges associated with addressing the global problems of the environment and with providing energy for society in a sustainable way. The articles in this publication indicate that rapid technological progress in the areas of energy generation, distribution and storage may change how we live today and lead to a sustainable way of life for future generations. Achieving this at the scale needed to make a real difference will require societal action at a level never before seen. New scientific innovation must be adopted, creating new and improved technologies that are more efficient, greener, cost competitive and socially responsible. This is true for both



Cover Image, "Harnessing Materials for Energy," MRS Bulletin Vol. 33, No. 4 (2008). Reproduced by permission of the MRS Bulletin.



Source: EIA Annual Energy Review 2007, AEO 2008

established energy technologies, such as fossil fuels, as well as renewable energy sources, such as wind and solar. The pie chart shows the contribution of renewable technologies to the United States' electricity generation capacity. Only 9.9% of this country's electricity was generated from renewable sources. The bulk of that, 7.1% of total electrical production, was generated by established hydroelectric power. Clearly there is room for increasing energy production from renewable sources. If we take global warming into consideration, however, it is an immense challenge to adopt renewable energy quickly enough to make a difference. For renewable energies to become a

significant part of our energy mix, considerable scientific and technological breakthroughs across a broad range of technologies (including energy generation, storage, transmission, and use) must be made and implemented. The entire spectrum of energy alternatives includes more efficient vehicles, lighting, electronics, and agricultural practices, as well as improved heating and cooling systems.

Much the same set of arguments can be used to defend the idea that not only energy and the environment, but also our health care system, has reached a tipping point. Just as our energy system requires transformation, our current health care system is also unsustainable. Fortunately, as in the case of energy production, new science and technologies for improving health care are emerging. From efforts ranging from the mapping of the human genome, to stem cell research, to gene therapy that will redefine the nature and expectations of health care worldwide, researchers are making steps, big and small, which will ultimately transform the life sciences.

The concurrence of several tipping points may permit changes in energy and health care to spread worldwide in an unprecedented way and allow an accelerated introduction of new technologies. Investments in the development of new science and technology can spur progress in a way that has not been seen since the Manhattan Project or the Moon Landing. This time however, we are not focused on one specific goal but on an integrated effort over a broad range of technologies, each with myriad significant goals.

Undergraduates, like those whose work is highlighted in this Journal, have the opportunity to be the catalysts of this change. By their actions and those of their classmates, they will provide the stimulus that drives the large scale implementation and adoption of new transformative technologies that lead to a sustainable way of life.

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21ST CENTURY SCIENCE IN A COMMUNICATION AGE

A solitary male wearing a white lab coat and holding a pipette sits on a stool by a counter festooned with beakers, test tubes and Bunsen burners; this persistent image of a scientist, toiling in isolation, bears almost no resemblance to scientific research as it is practiced today. Neither does it portray the authors of the research published in the following pages. On the contrary, the scientific research represented in this journal reflects the work of a diverse group of scientists consisting of undergraduate students and accomplished laboratory scientists working together on collaborative research teams. The papers and abstracts published here result from group efforts that reflect a scientific community where researchers are surrounded by colleagues and new communication tools: PDAs, computers, smart phones, web cams etc. — that represent a new world order, a scientific communication society.

One characteristic of science is that it is “creative,” i.e., the product of human intellect. A second characteristic is that science is “developmental,” i.e., never proven in the absolute or final sense, but always evolving. As a creative human and humanistic endeavor, the practice of science relies on quality communication, the efficient and accurate transfer of information — questions, ideas, hypotheses, observations, conclusions and theories — both among scientists themselves and between scientists and the society they hope to serve and advance. In recent years, radical new technologies that change the way we communicate are transforming how science is practiced, who practices science and the pace at which it is advancing.

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hypotheses, observations,
conclusions and theories
— both among scientists
themselves and between
scientists and the society*

Today, scientists, as well as the general public, enjoy instant access to scientific journals and papers as more and more authors' works are readily available online. This, along with media innovations such as YouTube, podcasts, webinars, wikis, online courses and blogs have added to the popularization of science, enhanced the ability of scientists to explain their findings to a lay audience, and made it possible for almost anyone to understand even the most arcane topics. Experts in highly specialized fields can communicate freely without regard for time or distance, making quality peer review and increased collaboration possible. Shared and combined data sets enhance and expand the evidence for existing theories and aid in the search for new ones. For the younger generation, often characterized as “digital natives,” utilizing the powers of these new communication tools is second nature. Their work, published here, provides evidence of scientific research aided and abetted by just such recent communication advances.

It is important to note, however, that in contrast to the positive aspects that new communication tools bring to the practice of science are real issues of intellectual property and authenticity of results. With self-publication available to anyone with Internet access comes increased opportunities to falsify and misrepresent results. Increased

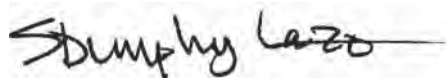
cross-cultural collaboration requires extra care to guard against the miscommunication and misinterpretations that may be inherent in such discourse. And the accelerated pace of scientific interchange encourages some to forego the careful deliberation still needed for the testing and retesting of theories and for guarding against the unintended consequences that rapid advances can bring.

Experts in highly specialized fields can communicate freely without regard for time or distance

Of course, individuals have never practiced science in a vacuum, and history is rich with examples of fruitful collaborative efforts. Today, however, the scientific community is at once more widespread and closer than ever before. The opportunities for collaboration are unprecedented and the mythological days of the solitary scientist restricted by geography and cumbersome communication tools are long since past. Paradoxically, just as advanced communication tools are seemingly shrinking our globe, they are expanding our scientific horizons. There is strong cause for hope that with the networking and information capabilities

available today, science as it is now practiced will achieve the kinds of transformational scientific breakthroughs that are needed to solve today's critical problems of global proportion.

Co-editors,



Shannon Dunphy Lazo, and



Lorna T. Vázquez, NBCT

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About the Cover

Transformational Science has the potential to change our entire view of the world overnight. The illustrations on the cover of this issue reflect current research efforts at the U.S. Department of Energy's (DOE's) National Laboratories that may lead to transformational changes in the way we see the world.

The DNA helix and the black cottonwood poplar tree represent the mapping of the *Populus trichocarpa* genome by students and researchers, just one example of the progress being made in nanoscience and genomics. Particle accelerators, the backbone of the physical sciences at DOE, alter scientists' understanding of the composition of the universe and the fundamental laws of physics. Images of solar panels and wind turbines highlight ongoing investigations into alternate sources of energy.

Relativistic Heavy Ion Collider tunnel image courtesy of Brookhaven National Laboratory.

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EDUCATING THE NEXT GENERATION OF SCIENTISTS AND ENGINEERS

U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE,
OFFICE OF WORKFORCE DEVELOPMENT FOR TEACHERS AND SCIENTISTS

Mentored Research Internships for College Students

Each year more than 600 undergraduate students are awarded paid internships at the Department of Energy's (DOE) National Laboratories. These interns are paired with research scientists who serve as mentors in authentic research projects. All participants write a research abstract and present at a poster session and/or complete a full-length research paper. Abstracts and selected papers from our 2007–2008 interns that represent the breadth and depth of undergraduate research performed each year at our National Laboratories are published here in the *Journal of Undergraduate Research*.

Interns are supported through one of the following four DOE programs.

Student Undergraduate Laboratory Internship (SULI)



This Program is open to university and community college students considering a career in science and/or engineering for summer, spring or fall sessions. Students who complete this internship gain first hand experience in a variety of STEM fields and are better able to understand the opportunities available to them in these fields.

Community College Institute (CCI) of Science and Technology



Students from community colleges can participate in this internship for science, engineering and technology at any of several different laboratories. In addition to their research, students in the program attend career planning and training/informational sessions.

Faculty and Student Teams (FaST)



This program is designed for faculty members and two or three undergraduate students from colleges and universities that receive below the 50th percentile in federal research funding as well as institutions serving populations underrepresented in the fields of science, engineering, and technology. These teams perform cutting-edge research as they partner with researchers at the laboratories. Continuing research grants are also available through this program.

Pre-Service Teacher Program (PST)



This program provides a rich experience for undergraduate students who are preparing to become K-12 science, technology, engineering or math teachers. Future teachers are paired with a master teacher and a laboratory scientist. Workshops for PST participants focus on bridging the gap from research to the classroom, offering suggestions on effective techniques to apply resources and translate the research experiences to students.

For more information on the above WDTS Programs, please contact helpwithapplication@science.doe.gov.

Many of the DOE National Laboratories have their own educational programs that are run locally or regionally. For information regarding these programs, please visit <http://science.doe.gov/feature/WDTS-map/WDTS-map.htm>.

Information regarding the science done at each laboratory is also available from individual websites. For a link to a listing of these websites, please visit http://www.science.doe.gov/National_Laboratories/index.htm.

Mohammad Moin Baig, from New York City, NY, received his bachelor's degree in 2008 from Medgar Evers College. He was selected to the FaST program for the summer of 2008 and worked on protein crystallization at Brookhaven National Laboratory. Mohammad presented a poster on this research in the DOE Science and Energy Research Challenge (SERCh) competition in Oak Ridge, Tennessee in November 2008. He is interested in learning more about structural genomics and pursuing studies in molecular biology. Mohammad's hobbies include working out, watching movies, and playing ping pong and cricket.

Ann C. Brown received a B.S. degree from Oakwood College, where she majored in biology with minors in chemistry and history. She received a master's in microbiology from the University of New Hampshire and a Ph.D. in anatomy/cell biology from New York Medical College. She currently is a professor in the biology department at Medgar Evers College. For the last two summers, Dr. Brown mentored two FaST students in the lab of Dr. Swaminathan at Brookhaven National Laboratory working on protein crystallization and X-ray crystallography.

S. Eswaramoorthy is a scientist at Brookhaven National Laboratory (BNL). He studied X-ray crystallography and biophysics at the University of Madras, India, and later moved to the Indian Institute of Science to learn macromolecular crystallography. He was a postdoctoral research associate at Ohio State University for a brief period, where he worked on nucleic acid structures. Dr. Eswaramoorthy joined BNL in 1998 with a background in structural biology.

S. Swaminathan graduated from the University of Madras, India, where he studied biophysics and crystallography. Before joining Brookhaven National Laboratory, he was a scientist at Veterans' Medical Center in Pittsburgh, PA. Dr. Swaminathan is currently a biophysicist in the biology department of BNL. His major interest is in structure-function relationships of proteins, especially toxins. He is a member of the New York Structural GenomiX Consortium funded by the Protein Structure Initiative of the National Institutes of Health (NIH) and leads the group at BNL.

CRYSTAL STRUCTURE ANALYSIS OF A PUTATIVE OXIDOREDUCTASE FROM *KLEBSIELLA PNEUMONIAE*

MOHAMMAD BAIG, ANN BROWN, S. ESWARAMOORTHY AND S. SWAMINATHAN

ABSTRACT

Klebsiella pneumoniae, a gram-negative enteric bacterium, is found in nosocomial infections which are acquired during hospital stays for about 10% of hospital patients in the United States. The crystal structure of a putative oxidoreductase from *K. pneumoniae* has been determined. The structural information of this *K. pneumoniae* protein was used to understand its function. Crystals of the putative oxidoreductase enzyme were obtained by the sitting drop vapor diffusion method using Polyethylene glycol (PEG) 3350, Bis-Tris buffer, pH 5.5 as precipitant. These crystals were used to collect X-ray data at beam line X12C of the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL). The crystal structure was determined using the SHELX program and refined with CNS 1.1. This protein, which is involved in the catalysis of an oxidation-reduction (redox) reaction, has an alpha/beta structure. It utilizes nicotinamide adenine dinucleotide phosphate (NADP) or nicotine adenine dinucleotide (NAD) to perform its function. This structure could be used to determine the active and co-factor binding sites of the protein, information that could help pharmaceutical companies in drug design and in determining the protein's relationship to disease treatment such as that for pneumonia and other related pathologies.

INTRODUCTION

Brookhaven National Laboratory (BNL), a U.S. Department of Energy (DOE)-sponsored research center located in Long Island, NY, provides research opportunities for scientists who conduct advanced research. A major interest of study at the BNL Structural Biology Laboratory is the determination of the crystallographic structure of bio-medically important target-proteins obtained from the New York GenomiX Research Consortium (NYSGXRC), a collaborative initiative with several major universities and research institutes. The research focus area at this laboratory is to use the three-dimensional structure of the target proteins to determine their functions [1]. The three-dimensional structure of a protein follows

the theory of evolution, which predicts the homology of specific proteins. Proteins that show similar amino acid sequences have evolutionary commonalities and form large families of proteins with common characteristics. "By studying protein folds and families, scientists are able to reconstruct the evolutionary relationship between two species and to estimate the time of divergence between two organisms, since they last shared a common ancestry" [2]. Once the three-dimensional structure is determined, researchers can decipher the family of that specific protein based on the atomic configuration.

Klebsiella pneumoniae is a gram-negative bacterium and produces an enzyme, a putative oxidoreductase, which belongs to a family of oxidoreductases that catalyze the transfer of electrons

from one molecule to another [3]. In this study, we first produced the required crystals of the enzyme and then used them to collect X-ray diffraction data at BNL's National Synchrotron Light Source (NSLS). The data were used to determine the three-dimensional structure of the protein.

MATERIALS AND METHODS

Purified protein was provided by the NYSGXRC consortium. It was crystallized using the sitting drop vapor diffusion method as follows. A droplet containing equal volumes (2 μ l each) of purified protein and a precipitant was allowed to equilibrate against a large reservoir (100 μ l) containing the same precipitant. Initially the droplet of protein solution contained an insufficient concentration of precipitant for crystallization, but as water vaporized from the drop and transferred to the reservoir, the precipitant concentration in the droplet increased to a level optimal for crystallization. Once the system was in equilibrium, these optimal conditions were maintained until the crystallization was complete [4]. After obtaining the initial crystallization condition, crystals of this protein were obtained using the precipitant containing 0.1 M Bis-Tris pH 5.5; 25% w/v polyethylene glycol (PEG) 3350, mixed with 10 mg/ml of protein sample at a 1:1 ratio (1:1 μ l) in the crystallization well and equilibrated against 100 μ l of the precipitant. The protein crystals obtained are shown in Figure 1. Crystals of the protein were then bombarded with X-rays to obtain diffraction intensity data used in structure determination.

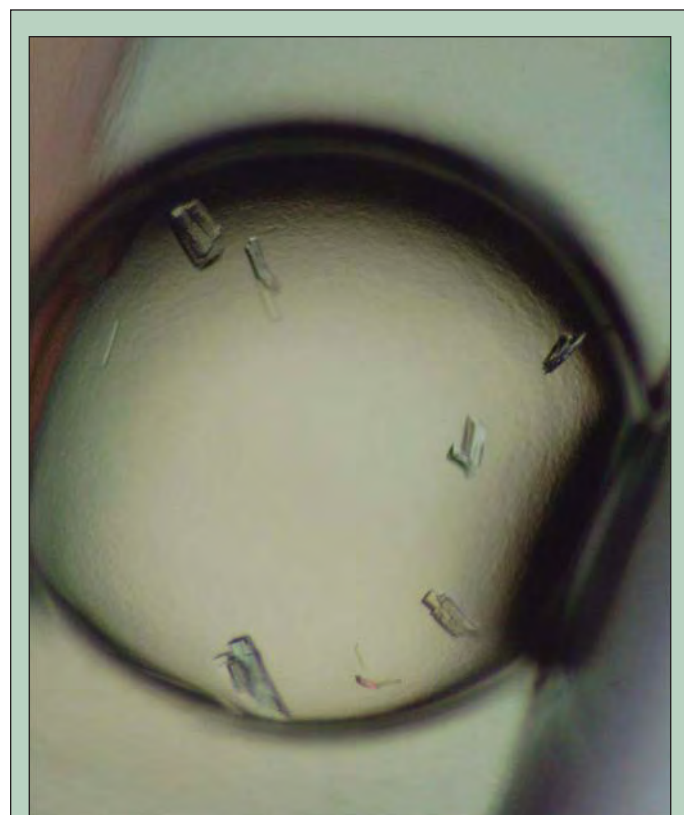


Figure 1. Crystals of the target protein. Crystals were formed in a solution containing 0.1 M Bis-Tris pH 5.5; 25% w/v polyethylene glycol (PEG) 3350 and 10 mg/ml of protein sample.

Crystals were flash frozen in liquid nitrogen using glycerol as cryoprotectant. Diffraction data at liquid N₂ temperature were collected at beam line X12C using a single wavelength (0.9795 Å) X-ray beam. The crystal diffracted to a resolution of 2.0 Å. The CBASS program was used to collect data and processed with HKL2000. Crystal parameters and data collection details are shown in Table 2. The selenium position of the protein was obtained by Single Anomalous Dispersion (SAD) method using the SHELX program and phase calculation and refinement was carried out with SHARP as shown in Table 1. The protein model was built using a model building program, ARP/wARP, and a graphics program, O. Coordinates for this structure are deposited to the Protein Data Bank (Id. code: 3E82).

Protein Purification
Crystallization → Sitting drop method
Data Collection → NSLS beam line X12C
Data Processing → HKL2000
Structure Solution → SHELX
Phase Refinement → SHARP
Protein Model Building
Structure Refinement and Analysis

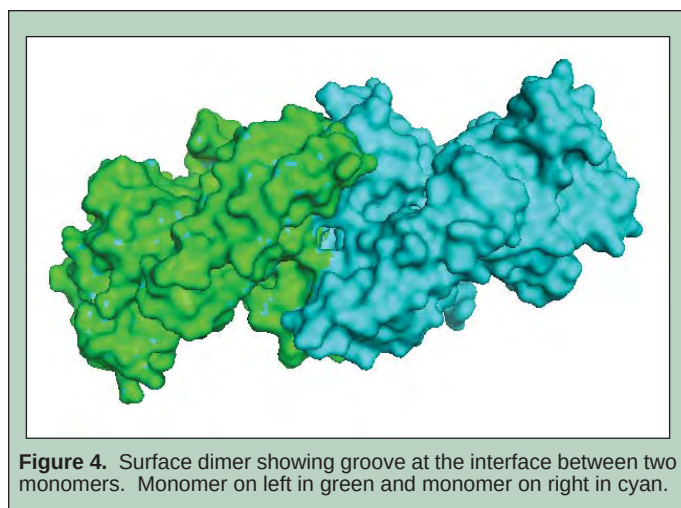
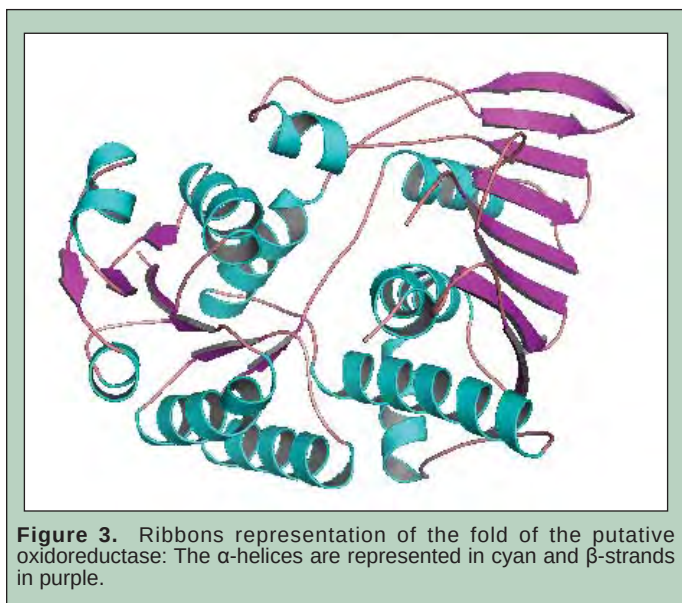
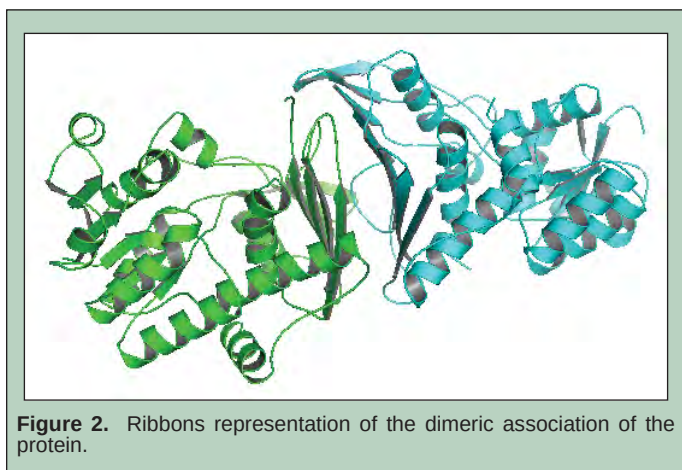
Table 1. Chart of protein structure determination procedure.

Number of crystals	1
X-ray source	Synchrotron (Beamline X12C)
Wavelength	0.9795 Å
Space group	P2 ₁
Unit cell parameter	a= 52.910 Å α = 90° b= 79.750 Å β = 93.99° c= 209.144 Å γ = 90°
Resolution	2.04 Å
R-merge	0.096
Unique number of reflections collected	109371
Percentage of completeness	98.8
Redundancy	7.5
Protein molecular weight	40 kDa
Number of residues of the protein	364
R value (working set)	0.209
Free R value	0.232
RMS deviations from ideal values	
Bond lengths (Å)	0.006
Bond angles (°)	1.30

Table 2. X-ray diffraction data.

RESULTS AND DISCUSSION

The crystal structure of the protein has been determined by the SAD method. This protein has selenium-substituted methionine (Se-Met) to facilitate anomalous dispersion data collection at the Se edge that is essential to determine the crystal structure. The crystal belongs to a monoclinic system ($P2_1$) and has two dimers in the crystallographic asymmetric unit, shown in Figure 2. The protein structure shown in Figure 3 represents the monomer. The molecule has a TIM barrel-like fold with eight helices at the outer circle and six strands inside. Sequence comparison of this 40 kDa protein shows more than 50% identity with many oxidoreductase proteins. These proteins should utilize NADP or NAD as cofactors, however this structure showed none. Still, when the dimers were examined carefully, a groove was observed on one side which is visible in Figure 4. This groove is a potential site where a molecule like NAD could reside. Further experiments with a complex of this protein with NAD or NADP may reveal the mode of cofactor binding. In addition, a cavity exists on the other side of the observed groove that is covered with charged residues such as Arg128, Glu322 and Arg137. This site may accommodate a substrate. More work has to be done to characterize the functional mechanism of this protein.



CONCLUSION

K. pneumoniae is a gram-negative bacteria that causes infection in the human intestinal tract, especially in hospital patients. The crystal structure of a putative oxidoreductase from this bacterium showed a TIM barrel fold and revealed the active site and co-factor binding sites. The three-dimensional structure of the protein plays a vital role in the protein's interaction with other molecules. This information can be used by pharmaceutical companies to design drugs that can be used to inhibit the activity of this particular protein.

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REMOTE DETECTION OF RADIOACTIVE PLUMES USING MILLIMETER WAVE TECHNOLOGY

ROSS BARNOWSKI, HUAL-TE CHIEN AND NACHAPPA GOPALSAMI

ABSTRACT

The reprocessing of spent nuclear fuel, a common method for manufacturing weapons-grade special nuclear materials, is accompanied by the release of fission products trapped within the fuel. One of these fission products is a radioactive isotope of Krypton (Kr-85); a pure β^- emitter with a half-life of 10.72 years. Due to its chemical neutrality and relatively long half life, nearly all of the Kr-85 is released into the surrounding air during reprocessing, resulting in a concentration of Kr-85 near the source that is several orders of magnitude higher than the typical background (atmospheric) concentrations. This high concentration of Kr-85 is accompanied by a proportionately high increase in air ionization due to the release of beta radiation from Kr-85 decay. Millimeter wave (MMW) sensing technology can be used to detect the presence of Kr-85 induced plumes since a high concentration of ions in the air increases the radar cross section due to a combination of atmospheric phenomena. Possible applications for this technology include the remote sensing of reprocessing activities across national borders bolstering global anti-proliferation initiatives. The feasibility of using MMW radar technology to uniquely detect the presence of Kr-85 can be tested using commercial ion generators or sealed radioactive sources in the laboratory. In this paper we describe our work to derive an ion dispersion model that will describe the spatial distribution of ions from Kr-85 and other common lab sources. The types and energies of radiation emitted by isotopes Co-60 and Cs-137 were researched, and these parameters were incorporated into these dispersion models. Our results can be compared with the results of MMW detection experiments in order to quantify the relationship between radar cross section and air ionization as well as to further calibrate the MMW detection equipment.

INTRODUCTION

With the incredible potential for destruction attributed to nuclear weapons, the proliferation of special nuclear materials (SNM) is a notable concern for both national and global security. One possible method by which SNMs can be manufactured is the reprocessing of spent nuclear fuel. In fact, some reactors are designed specifically to enhance plutonium production for the purpose of bolstering nuclear weapons programs [1]. When nuclear fuel is reprocessed, fission products trapped within the fuel are released. One of the most prominent gaseous fission products is Krypton-85 (Kr-85), which is created in abundance in typical fission reactions. Kr-85 has a half-life of over 10 years, so it will not decay during the 1–2 year fuel-storage period that is typical before reprocessing occurs. Additionally, since Krypton is a noble-gas, it does not readily chemically react making it very difficult to suppress emissions of the gas during the reprocessing procedure [2]. Furthermore, Kr-85 is radioactive; a pure β^- emitter with an average energy of 251 keV/particle [3]. Studies have shown [4] that emissions of Kr-85 during reprocessing exceed the background (atmospheric) concentrations of the isotope by several orders of magnitude. Therefore, detection of Kr-85 offers a pragmatic and unique method for detecting the reprocessing of nuclear fuel.

Currently, the only way to detect the presence of Kr-85 is via atmospheric sampling [4]. Although effective under certain circumstances, this method has several drawbacks. First, collection efficiency is greatly affected by uncontrollable parameters such as wind, rough terrain and national borders. Wind and terrain can dramatically affect where and how far the plume of radioactive Kr-85 will spread. Furthermore, the detection efficiency decreases as distance from the source increases, so national borders impose a significant hurdle to international Kr-85 detection for nuclear fuel reprocessing plants far from borderlines. Additionally, it is neither practical nor cost-effective to continually sample the atmosphere, which limits the atmospheric collection method to applications where the time-frame of Kr-85 emissions is known. Ideally the disadvantages of the atmospheric collection method can be eliminated by using MMW radar to detect Kr-85 emissions directly near the source (the stack of a reprocessing plant).

The ability to cheaply and continuously monitor the output of known and suspected reprocessing facilities will greatly enhance the ability of international organizations to monitor compliance with non-proliferation treaties and initiatives. Rather than detect Kr-85 directly, the MMW radar will detect the ionized air that results from the emission of radioactive Kr-85. Ionized air has a higher radar cross-section than normal air, which allows plumes of radioactive gasses to be distinctly imaged or detected. Furthermore, other atmospheric phenomena such as ion-induced nucleation can further increase the radar cross-section of such plumes. These "tell tale" signatures in combination with the a priori knowledge of the plant and weather conditions would then indicate the presence of Kr-85, uniquely proving that fuel was being reprocessed. The goal of this project is to develop models for the spatial dispersion of ions, which can be used as a benchmark to test and calibrate the MMW system.

Centimeter-wave technology has been previously used to image the emissions of several commercial power plants [5]. However, the

physical process by which radar cross section is increased due to radiation-induced ion concentration is complicated and, currently, not well understood. In the absence of a model that predicts radar cross section based on air ion concentration, experiments must be designed to test the response of the MMW technology to different sources and concentrations of ions. Therefore, it is important to derive models to predict the spatial distribution and concentration of ions from different sources so that the results of the experiments can be benchmarked.

MATERIALS AND METHODS

Isotopes of Interest

The release and decay of Kr-85 is the most significant contributor to the increase in air ion concentration [2] during a reprocessing event. In fact, calculations using data from a study on reprocessing has shown that the ion concentration due to Kr-85 decay is expected to be three or more orders of magnitude greater than the atmospheric ion concentration [4]. However, Kr-85 is not an easily obtainable source for use in the laboratory due to the fact that its gaseous nature presents a significant health risk to laboratory personnel. Alternate sources such as Co-60 and Cs-137 are available from many vendors in the form of sealed disk sources, making them convenient for laboratory use. Although the types and energies of the radiation emitted from each of these sources differ from Kr-85, these sources are useful to study the MMW interaction of air ionization that occurs and the spatial distribution of those ions.

There are several parameters of interest in the construction of a spatially-dependent ion model, such as the path length of a typical beta particle (with given energy); the average number of ion pairs formed per energy of a beta particle; and contributions from gamma radiation. All of these parameters have a distinct affect on the derivation of a spatial ion model, and need to be taken into account for each of the individual isotopes. The energy spectra and decay modes of Kr-85, Co-60 and Cs-137 are well known, and all of the pertinent data for each of these isotopes can be found in references [3], [6] and [7] respectively.

Estimate of Radiative Losses for Given Beta Particles

Since ion pair formation is the main concern for this application, energy losses through non-collisional pathways such as Bremsstrahlung must be accounted for. Radiative losses such as Bremsstrahlung represent energy loss mechanism that do not directly form ion pairs and hence detract from the formation of an ion plume. The actual ratio of radiative to collisional energy loss is a complex expression; however the following expression gives an accurate approximation.

$$\frac{(dE/dx)_r}{(dE/dx)_c} \approx \frac{EZ}{700} \quad (1)$$

where E is energy in units of MeV, and Z is the atomic number of the medium through which the β^- travels. The derivative terms on the left hand side of Eq. (1) represents the ratio of radiative stopping power to the collisional stopping power. Integrating Eq. (1) over all space yields the ratio of total radiative energy loss to total collisional energy loss for a particle of known energy. This approximation is used for each of the isotopes, Co-60 and Cs-137. In order to ensure the estimate is conservative, the maximum β^- energies will be used for E and the highest possible value will be used for Z. Since the

medium of interest is air, which is composed of ~78% nitrogen (Z=7) and 22% oxygen (Z=8), a value of Z=8 will be used.

The results of the calculation for each of the three isotopes are shown in Table 1, and clearly indicate that the amount of energy lost to Bremsstrahlung for each of the three isotopes is negligible. These data are supported by the following conceptual argument: since the kinetic energy of the β^- particle is relatively small, the amount of energy lost in the event of an inelastic collision would likewise be negligibly small. Therefore, it can be assumed that all of a given β^- 's energy is lost to the formation of ions in atmospheric air.

Isotope	Maximum Beta Energy (MeV)	$\frac{(dE/dx)_r}{(dE/dx)_c}$
Kr-85	0.6874	0.7856%
Co-60	0.3182	0.3637%
Cs-137	0.5140	0.5874%

Table 1. Table showing conservative estimates for the total percentage of energy lost to Bremsstrahlung for each of the three isotopes of interest.

Ion Pairs per Beta Particle

The previous section demonstrated that the beta particles from Co-60, Cs-137 and Kr-85 lose all of their energy to the formation of ion-pairs in air. The number of ion pairs corresponding to a typical β^- from each isotope can be calculated. This is an important input parameter for the spatial ion-distribution model, describing the number of ion-pairs expected to be produced per charged particle. It will be assumed that a β^- emitted by a particular isotope has a kinetic energy equal to the average kinetic energy of the spectrum for that isotope. The W-value for air is 33.8 eV/ion-pair [8].

Using this information, the average number of ion pairs created per β^- can be calculated as:

$$\frac{\text{Avg eV}}{\beta^- \text{ particle}} \div (W\text{-value}) \left(\frac{\text{ion pairs}}{\text{eV}} \right) = \frac{\text{ion pairs}}{\beta^- \text{ particle}} \quad (2)$$

The information in Table 2 can be used to verify a value for the expected number of ion-pairs created per m³ per second by Kr-85 emissions from reprocessing plants. A study from the WAK reprocessing facility in Germany gives a value of 2.7 mCi/m³s due to Kr-85 emission during reprocessing [4]. Using this data, the number of ion pairs/cm³s can be calculated:

$$\begin{aligned} & \frac{2.7 \text{ mCi}}{\text{m}^3} \times \frac{3.7 \times 10^{10} \text{ Bq}}{1000 \text{ mCi}} \times \frac{1 \beta^- / \text{sec}}{1 \text{ Bq}} \times \frac{7443 \text{ ion pairs}}{1 \beta^-} \\ &= \frac{7.4 \times 10^{11} \text{ ion pairs}}{\text{m}^3 \text{ s}} = \frac{7.4 \times 10^5 \text{ ion pairs}}{\text{cm}^3 \text{ s}} \quad (3) \end{aligned}$$

Isotope	Avg Beta Energy (eV)	Avg # Ion Pairs/ Beta Particle
Kr-85	251590	~ 7443
Co-60	95770	~ 2833
Cs-137	174320	~ 5157

Table 2. Table showing the expected average number of ion pairs produced in air per beta particle from each of three sources of interest.

The specific production rate of ions due to Kr-85 emissions of the given activity is roughly 7.4×10^5 ion-pairs/cm³s. This value can serve as a baseline for experiments where the ion production parameter can be controlled.

A couple of points should be noted about Eq. (3). First, it is assumed that ion pairs are created instantaneously coinciding with the release of a β^- . The β^- has a velocity near the speed of light when released, and its maximum travel length never exceeds three meters as per rule of thumb. Since time = distance/velocity, to a classical approximation, this assumption is valid.

Another more egregious omission is the recombination of ions once they are formed. Models of this process are currently underdeveloped and go beyond the scope of this study, but it is expected that such models will be useful in the future.

Maximum Beta Particle Range in Air

The range of the β^- in air is an important parameter because it represents the distance over which significant ionization is expected to occur. The definition of maximum range of a β^- assumes that the particle traveled in a straight line, although this is rarely ever the case. It has been found that the range is largely a function of the β^- energy, and the density of the medium material, regardless of the material's other properties [8]. Figure 1 illustrates this fact and is used to derive expected values for the range of the β^- 's emitted by each of the above three isotopes. In this case, we will estimate the range x density values for the average energy and the maximum energy of a β^- from each of the three sources. The results can be found in Table 3.

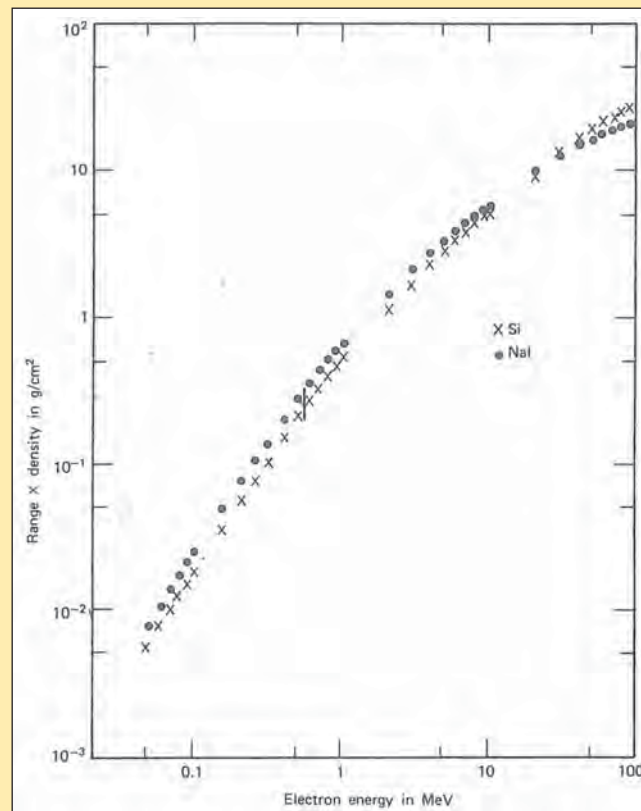


Figure 1. Figure showing the range x density value for several materials as a function of beta particle energy. Notice that the figure shows the trend is relatively constant regardless of which material is considered [8].

Isotope	Max Beta Energy (MeV)	Avg Beta Energy (MeV)	Maximum Estimated Range*Density (g/cm ²)	Average Estimated Range*Density (g/cm ²)	Max Est. Range (cm)	Avg Est. Range (cm)
Kr-85	0.6874	0.25159	0.3	0.06	232.0	46.4
Co-60	0.3182	0.09577	0.1	0.015	77.3	11.6
Cs-137	0.514	0.17432	0.11	0.028	85.1	21.7

Table 3. Estimates of the average and maximum range of the beta particles in air based on the range x density plot (Figure 1). The maximum and average energies of the beta particles were used to determine corresponding "maximum" and "average" range x density values on the chart above. To calculate the range, the range x density values were simply divided by the density of dry air, approximately 0.001293 g/cm³.

Gamma Ray Interaction in Air

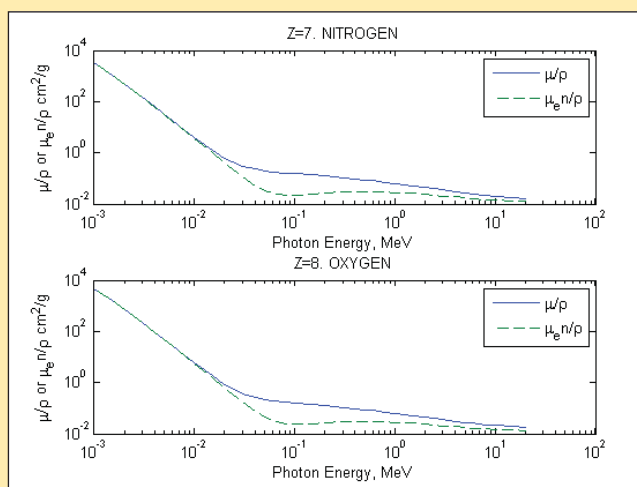
Although Kr-85 is a pure beta emitter, the sources that will likely be used in the lab emit both beta and gamma radiation. For instance, some common lab sources, including Cobalt-60 (Co-60) and Cesium-137 (Cs-137), are dual gamma and β^- emitters. Therefore, it will be useful to know what effect, if any, the gamma radiation will have on ionization.

The probability of a gamma ray interaction in any medium is measured with an attenuation coefficient, μ , which is the probability, per unit path length, that a gamma-ray photon will be removed from a theoretical beam defined by its initial path [8]. The attenuation coefficient is dependent on the energy of the gamma ray, the atomic number of the medium, and the density of the attenuating material. Since the medium of interest in this case is air, we are interested in the attenuation properties of nitrogen and oxygen under reasonable atmospheric conditions. The mass attenuation coefficient (which accounts for density) can be estimated from published graphs and Tables (Graph A, [9] and Table 4).

The density of dry air at standard atmospheric conditions is about 0.001293 g/cm³ [8]. Using this value for the density, we can calculate the probability per unit path length of an interaction between the gamma ray and the medium. An alternate way to characterize the same property is to calculate the mean free path of the gamma ray in the given medium. The mean free path is defined as the average distance that the gamma ray travels through the medium before any interaction takes place. This value is simply the reciprocal of the attenuation coefficient and is shown in Table 5.

The values for mean free path length for gamma rays from Co-60 and Cs-137 are ~160 m and ~85 m respectively. As rough estimates, even if they are an order of magnitude too high, these values still show that the gamma rays interact far less in air than beta particles do. Hence the ion production rate from gamma rays is expected to be much smaller than that from beta particles. However, in a laboratory setting, the gamma rays are bound to hit other solid materials/equipment and emit secondary energetic electrons which will cause ionization in air like beta particles do. See Eq. (4) for an estimate of ion production rate as a function of distance from a gamma ray source of given activity.

Each of these calculated parameters plays a role in the spatial ionization model. The amount of ions produced per beta particle and the maximum beta particle range help define the magnitude and spatial resolution of the models, respectively. The gamma-ray range in air similarly plays a role in determining the spatial scale of the model. Finally, the calculated absence of radiative losses allows the model to ignore loss terms due to Bremsstrahlung.



Graph A. Mass attenuation coefficients for nitrogen and oxygen.

Isotope	γ -Energy (MeV)	μ/p (cm ² /g) for O	μ/p (cm ² /g) for N	Est. μ/p (cm ² /g) for Air
Co-60	1.173, 1.332	0.035	0.05	0.0467
Cs-137	0.682	0.09	0.085	0.0861

Table 4. Table showing the estimates for the mass attenuation coefficient for gamma rays in oxygen, nitrogen and air. The oxygen and nitrogen values were estimated using the graphs found in Appendix A. The estimate for air is calculated by the following formula: $0.78 \times \text{N-value} + 0.22 \times \text{O-value}$. This is intended to compensate for the concentration of nitrogen and oxygen in air.

Isotope	Est. μ/p (cm ² /g) for Air	μ (1/cm)	λ (cm)
Co-60	0.0489	6.323E-05	1.582E+04
Cs-137	0.0927	1.20E-04	8.343E+03

Table 5. Table showing the calculated estimates for the mass attenuation coefficient and the mean free path of the gamma rays emitted by the two listed sources.

Spatial Ionization Models for Isotopes of Interest

The information calculated in the above section for Co-60 and Cs-137 was applied in the development of a model to calculate the expected amount of ionization from disk sources of Cs-137 and Co-60 of known activity as a function of distance from the source. These predicted values will then be compared to any measured changes in cross section to greater understand the relationship between ion concentration and changes in radar cross section. Co-60 and Cs-137 were considered for this ion model because these isotopes will most likely be used for laboratory tests of MMW technology. Furthermore, the results of these models could easily be extended to Kr-85 sources, since the principles used to derive the parameters in the calculations section do not differ for different isotopes.

RESULTS AND DISCUSSION

Since ionization is, by far, the most prevalent pathway by which gamma ray energy can lose energy in air, the measure of charge/unit mass (gamma source exposure rate) can easily be converted to ion-pairs/unit mass. The exposure rate equation is based on the assumption that the volume of interest is large compared to the size of the source (i.e., spherical geometry is applicable). Since the mean free path of the high energy gamma rays of interest is on the order of tens of meters in air, and since most lab sources tend to be small disk sources, this assumption is upheld quite well. The equation for calculating exposure rate from activity is given by Knoll [8] as:

$$X = \Gamma \frac{A}{d^2} \quad (4)$$

where,

X = exposure rate (R/hr)

Γ = the exposure rate constant ($R \cdot cm^2 / (hr \cdot mCi)$)

A = Activity (mCi)

d = straight-line distance from source to point of interest (cm).

Eq. (4) shows that exposure rate can be calculated as a function of distance if the activity and the exposure rate constant are known for the isotopes of interest. Exposure rate constants can be found in a number of radiological health resources [10], while the activity must be a given parameter. The parameters of interest for Co-60 and Cs-137 are given in Table 6.

Isotope	Exposure Rate Constant ($R \cdot cm^2 / (hr \cdot mCi)$)	Activity (mCi)
Cs-137	3.3	0.4
Co-60	13.2	0.95

Table 6. Exposure rate constants and activities for Cs-137 and Co-60. The exposure rate constants were looked up on page 59 of reference 8. The activities of the sources were specified by the designers of the experiment.

The conversion between Roentgen and ion-pairs per mass is: $1R = 2.08 \times 10^9$ ion-pairs/0.001293 g air (1 cm^3 at standard temperature and pressure (STP)) [8]. Therefore, if it is assumed that the medium is at STP, the value for exposure rate can be converted to ion-pairs/ cm^3/s ; which is the parameter of interest.

Carrying out the calculation for Co-60 and Cs-137 and then converting the answer to ion-pairs/ cm^3/s yields:

$$\begin{aligned} \dot{X} &= 13.2 \frac{0.4}{d^2} = \frac{12.6}{d^2} \frac{R}{hr} * \frac{1 hr}{3600 s} = 0.0035 \frac{R}{s} \\ &* \frac{2.08 \times 10^9 \text{ ion pairs/cm}^3}{1R} \Rightarrow \frac{7.28 \times 10^6 \text{ ion pairs}}{d^2 \text{ cm}^3 s} \end{aligned} \quad (5)$$

for Co-60 and

$$\begin{aligned} \dot{X} &= 3.3 \frac{0.4}{d^2} = \frac{1.32}{d^2} \frac{R}{hr} * \frac{1 hr}{3600 s} = 0.000367 \frac{R}{s} \\ &* \frac{2.08 \times 10^9 \text{ ion pairs/cm}^3}{1R} \Rightarrow \frac{7.63 \times 10^5 \text{ ion pairs}}{d^2 \text{ cm}^3 s} \end{aligned} \quad (6)$$

for Cs-137.

Therefore, given the distance in centimeters, the number of ion pairs produced per cm^3 of air as a result of gamma ray radiation is $7.28 \times 10^6/d^2$ ion pairs/ cm^3/s for Co-60 and $7.63 \times 10^5/d^2$ ion pairs/ cm^3/s for Cs-137. At a sample distance from the source of 10 cm, these equations yield 7.28×10^4 ion pairs/ cm^3/s for Co-60 and 7.63×10^3 ion pairs/ cm^3/s for Cs-137.

Unlike the gamma ray case, no convenient equation exists to calculate the amount of ionization as a function of the spatial distribution of the beta particles. In order to estimate the amount of ion-pair production as a function of spatial distribution, a simple spatial model will be derived based on the following assumptions.

1. Although beta particles are emitted with a spectrum of possible energies, it will be assumed that each beta particle emitted by the source leaves with the average energy for that particular spectrum (i.e., 95.77 keV for Co-60 and 174.32 keV for Cs-137).
2. Since the path of beta particles is erratic in air, the overall motion of any given beta particle will be characterized as random. It follows that the ion pairs due to beta radiation follows a Gaussian spatial distribution.
3. From the central limit theorem, it can be shown that 99.7% of the expected values will reside within three standard deviations of the mean for a normal distribution. In this case, the mean value is zero (in other words, the average value of the distance traveled is zero, since the emission of beta particles from the source is assumed to be spherically symmetric). Therefore, it will be stated that three standard deviations will correspond to the maximum range of a beta particle in air.
4. The magnitude of the distribution can be calculated in the following manner. Given the average number of ion pairs produced per beta particle as calculated above and the number of beta particles emitted per unit time which can be estimated by the activity of the source, the Cs-137 source is expected to emit $0.4 \times 3.7 \times 10^7 = 1.48 \times 10^7$ beta particles/second, while the Co-60 source is expected to emit $0.95 \times 3.7 \times 10^7 = 3.52 \times 10^7$ beta particles/second. Therefore, the number of ion pairs produced per second due to beta radiation is:

$$1.48 \times 10^7 \times 2833 = 4.19 \times 10^{10} \text{ ip/s for Co-60,}$$

$$\text{and } 3.52 \times 10^7 \times 5157 = 1.81 \times 10^{11} \text{ ip/s for Cs-137.}$$

The general form for a Gaussian distribution [11] is given by:

$$f(x) = \frac{A}{\sigma \sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right) \quad (7)$$

where A is the magnitude of the distribution, σ is the standard deviation, and x is the single spatial dimension considered. Calculating A and σ as described above, we are left with the parameters given in Table 7 for Co-60 and Cs-137.

Isotope	A (ip/s)	Max Range (cm) (from Table 3)	σ (cm)
Cs-137	1.18E+11	77.3	28.3
Co-60	4.19E+10	85.1	25

Table 7. Parameters A and σ for Cs-137 and Co-60 as calculated for the spatial ion model above.

It does not matter whether an ion pair was created indirectly by gamma ray interactions or by beta particle interactions. The total number of ion pairs at any given distance is expected to be the sum of the ion pairs created by gamma radiation and beta radiation. Thus, combining all of the information above, the spatially-dependent functions of ion density for each isotope is:

$$f(x[\text{cm}]) = \frac{A}{\sigma\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right) + \frac{7.08 \times 10^6}{x^2} \quad (8)$$

for Co-60, where

$$A = 4.19 \times 10^{10} \text{ ip/s;}$$

$$\sigma = 25 \text{ cm;}$$

$$x = \text{distance from source (cm);}$$

and

$$f(x[\text{cm}]) = \frac{A}{\sigma\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right) + \frac{7.63 \times 10^5}{x^2}; \text{ where}$$

$$A = 1.81 \times 10^{11} \text{ ip/s;}$$

$$\sigma = 28.33 \text{ cm;}$$

$$x = \text{distance from source (cm);}$$

for Cs-137.

CONCLUSION

Figures 2 and 3 show the results of these models plotted in two dimensions from which we can conclude that the contribution of ion pairs due to gamma radiation is negligible compared to the amount of ion pairs produced by beta radiation. This matches the prediction made above.

One of the shortcomings of this model is that it does not take into account recombination. The simplest models for recombination are often shown in differential form such that: $\frac{dn}{dt} = -\alpha * n^2$ where $n(t)$ is the concentration of ions and α is a recombination coefficient [5]. However, this model is not accurate in this case because the mechanisms for recombination in the atmosphere are far more complex than this model suggests. Also, values for α are not accurately known for situations where ion concentrations are higher than the general background level. Since recombination is not considered in the above model, the density of ions predicted by the model may be somewhat higher than what is observed. More research is needed to better understand the role of recombination in high-ion density atmospheric situations.

Also, notice that the ion-pair densities predicted by the model are given in ip/cm³s. The time dependence is a consequence of the activity of the sources. In a previous model it has been shown that

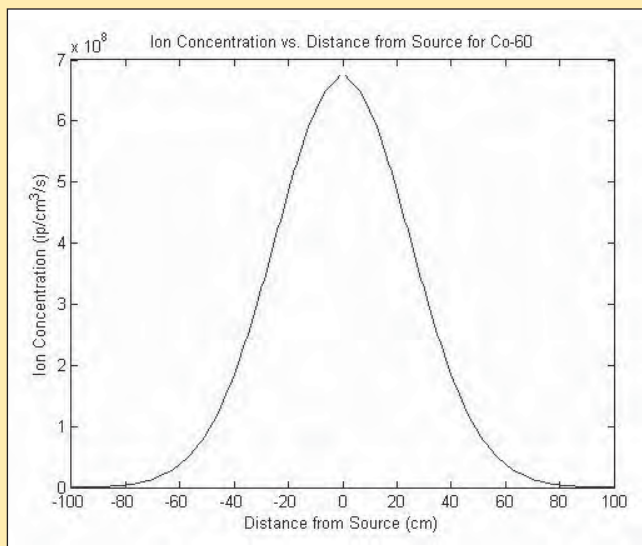


Figure 2. A figure showing the spatial distribution of ion pairs from the decay of a 0.95 mCi disk source of Co-60.

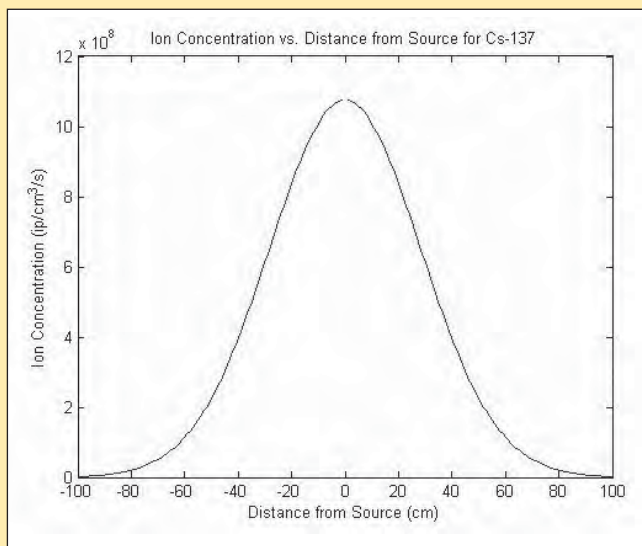


Figure 3. A figure showing the spatial distribution of ion pairs from the decay of a 0.4 mCi disk source of Cs-137.

the ion concentration tends to approach the value predicted by the time dependent model in a relatively short time frame. This indicates that after several milliseconds, the densities predicted by the model tend to be time independent. This is largely due to diffusion and recombination of ions.

Due to their ready availability, Co-60 and Cs-137 were identified as the most obvious choices for laboratory sources to be used to test and calibrate the MMW detection technology. Parameters such as the range of beta particles in air, the range of gamma rays in air, and the number of ion-pairs expected to be produced by each type of radiation were calculated. These parameters were then incorporated into a spatial ion model based on a Gaussian spatial distribution. The results of these models will be used as a starting point against which the detection data from MMW tests in the laboratory can be

checked. Currently, this model is based on generalized assumptions, and will be refined upon collecting data using the MMW detection system.

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CONTROLLED GROWTH OF CARBON NANOTUBES ON CONDUCTIVE METAL SUBSTRATES FOR ENERGY STORAGE APPLICATIONS

PATRICK BROWN AND CHAIWAT ENGTRAKUL

ABSTRACT

The impressive mechanical and electronic properties of carbon nanotubes (CNTs) make them ideally suited for use in a variety of nanostructured devices, especially in the realm of energy production and storage. In particular, vertically-aligned CNT "forests" have been the focus of increasing investigation for use in supercapacitor electrodes and as hydrogen adsorption substrates. Vertically-aligned CNT growth was attempted on metal substrates by water-assisted chemical vapor deposition (CVD). CNT growth was catalyzed by iron-molybdenum (FeMo) nanoparticle catalysts synthesized by a colloidal method, which were then spin-coated onto Inconel® foils. The substrates were loaded into a custom-built CVD apparatus, where CNT growth was initiated by heating the substrates to 750 °C under the flow of He, H₂, C₂H₄ and a controlled amount of water vapor. The resultant CNTs were characterized by a variety of methods including Raman spectroscopy, transmission electron microscopy (TEM) and scanning electron microscopy (SEM), and the growth parameters were varied in an attempt to optimize the purity and growth yield of the CNTs. The surface area and hydrogen adsorption characteristics of the CNTs were quantified by the Brunauer-Emmett-Teller (BET) and Sieverts methods, and their capacitance was measured via cyclic voltammetry. While vertically-aligned CNT growth could not be verified, TEM and SEM analysis indicated that CNT growth was still obtained, resulting in multiwalled CNTs of a wide range in diameter along with some amorphous carbon impurities. These microscopy findings were reinforced by Raman spectroscopy, which resulted in a G/D ratio ranging from 1.5 to 3 across different samples, suggestive of multiwalled CNTs. Changes in gas flow rates and water concentration during CNT growth were not found to have a discernable effect on the purity of the CNTs. The specific capacitance of a CNT/FeMo/Inconel® electrode was found to be 3.2 F/g, and the BET surface area of a characteristic CNT sample was measured to be 232 m²/g with a cryogenic (77K) hydrogen storage of 0.85 wt%. This level of hydrogen adsorption is slightly higher than that predicted by the Chahine rule, indicating that these CNTs may bind hydrogen more strongly than other carbonaceous materials. More work is needed to confirm and determine the reason for increased hydrogen adsorption in these CNTs, and to test them for use as catalyst support networks. This study demonstrates the feasibility of producing CNTs for energy storage applications using water-assisted CVD.

INTRODUCTION

Carbon nanotubes (CNTs), since their discovery in 1991 by Iijima [1], have been the subject of intense scientific inquiry and much media attention. CNTs consist of thinly rolled sheets of graphene with covalently bonded sp^2 carbon atoms arranged in a hexagonal network. Single-walled CNTs (SWCNTs) contain only a single graphene layer, but double-walled CNTs (DWCNTs) and multi-walled CNTs (MWCNTs) are also possible. CNTs, which have widths from less than a nanometer to hundreds of nanometers and lengths up to many millimeters, have a host of interesting and technologically useful properties [2]; they demonstrate high thermal [3] and electrical [4] conductivity, unique electronic structure [5], incredible tensile strength [6] and high surface area, making them ideal candidates for use in a variety of nanostructured devices. Single-walled CNTs also possess tunable band gaps depending on the orientation of their wrapping vector, and the preferential synthesis of semiconducting SWCNTs has recently been demonstrated [7].

Large-scale synthesis of CNTs is typically performed using such methods as arc discharge [8], laser ablation [9], or the high pressure carbon monoxide (HiPco) process [10]. These techniques are highly efficient and reproducible but tend to form disordered bundles of CNTs, which can be hard to fashion into useful devices. While the CNTs themselves still demonstrate high conductivity, disordered films of carbon nanotubes contain multiple grain boundaries in the form of gaps between the nanotubes, preventing the full realization of their ballistic electron transport. On the other hand, a promising and relatively new method of CNT growth, chemical vapor deposition (CVD), has been found to produce vertically-aligned carbon nanotube “forests” (VACNT) [11]. Individual CNTs extend through the entire height of these forests, which have been grown to heights of up to 7 mm [12], and demonstrate much denser packing than is achieved through other synthetic methods. In this case, the superb mechanical and electronic properties of CNTs can be utilized on a macroscopic scale, opening the door for their incorporation into next-generation devices.

Carbon nanotubes have been studied for use in a wide variety of applications, including organic transistors [13], organic LEDs [14], and chemical sensors [15]. CNTs have even been drawn into macroscopic ropes or sheets, which demonstrate tensile strength far surpassing that of ordinary macroscopically-organized materials [16]. Some of the most exciting new applications for CNTs lie in the realm of energy production and storage. CNTs have been shown to increase charge collection and transport in dye-sensitized [17] and quantum dot [18] solar cells, and have been used as conductive electrodes in organic photovoltaics [19], [20]. They have also been shown to have beneficial effects upon incorporation into fuel cell electrodes [21]. The high surface area and conductivity of CNTs also makes them ideally suited for use in supercapacitors [22]–[24]. Supercapacitors store charge in an electrical double layer formed between a high surface area electrode and an electrolyte, and may also display “pseudocapacitance” in the form of rapid faradaic charge transfer reactions involving redox-active components on the electrode surface. VACNTs grown directly on conductive metal substrates constitute a complete supercapacitor electrode and demonstrate much greater packing density and closer interaction with the contacts than conventional supercapacitors based on disordered carbon

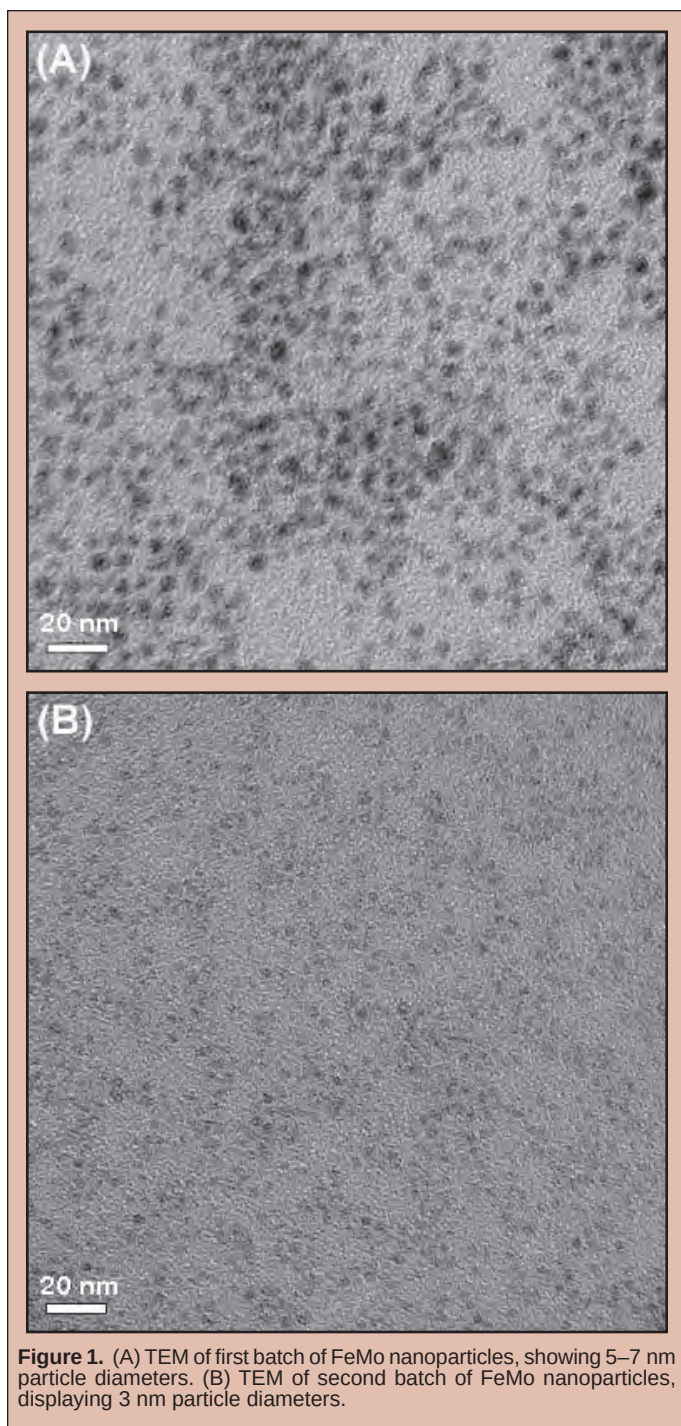
materials [25], [26]. Single-walled CNTs have also been shown to act as effective substrates for hydrogen adsorption [27], and the same properties that make VACNTs effective in supercapacitors should also apply to their use in hydrogen storage. In particular, the long-range order and highly accessible surface area of VACNTs should allow for faster and more complete hydrogen uptake, as well as easier incorporation of inorganic hydrogen dissociation catalysts.

In the present study, vertically aligned carbon nanotube growth by water-assisted chemical vapor deposition was attempted [11]. VACNT growth was catalyzed by iron-molybdenum (FeMo) nanoparticles synthesized by a colloidal method [28], [29] and deposited onto conductive metal substrates [30]. The resulting CNT forests were characterized by Raman spectroscopy [31], transmission electron microscopy (TEM) and scanning electron microscopy (SEM) to determine the purity of the nanotubes and the relative amounts of single-walled CNTs and multi-walled CNTs, and the growth parameters were varied in an attempt to optimize the yield of the CNT growth and to increase the purity of the CNTs present. The surface area and hydrogen adsorption characteristics of the nanotubes were quantified by the Brunauer-Emmett-Teller (BET) and Sieverts methods, respectively, and the specific capacitance was measured via cyclic voltammetry in an attempt to evaluate the potential of VACNTs for use in nanostructured energy storage devices.

MATERIALS AND METHODS

Colloidal Nanoparticle Catalysts

Colloidal FeMo nanoparticles were synthesized as was done by Nishino, et al. [29], with oleic acid as the protecting agent to prevent aggregation of the nanoparticles. Iron pentacarbonyl, molybdenum hexacarbonyl, oleic acid, octyl ether and 1-octadecene were all used as received. Two syntheses were performed. In the first synthesis, 0.03 g of oleic acid (0.10 mmol) was dissolved in 15 mL of 1-octadecene and heated to 220 °C while stirring under a He atmosphere in a 100 mL three-necked flask. The injection solution of 0.98 g $Fe(CO)_5$ (5.0 mmol) and 0.092 g $Mo(CO)_6$ (0.35 mmol) was mixed under inert atmosphere, then rapidly injected while vigorously stirring the hot reaction mixture. After injection, a large amount of gas evolved and the mixture changed from pale yellow to black, indicating decomposition of the metal complexes and formation of colloidal nanoparticles. The solution was heated for 30 min. at 220 °C, then annealed for 30 min. at 287 °C. After cooling, any large aggregates were removed by centrifugation. The nanoparticles were precipitated with anhydrous ethanol, centrifuged and redispersed in n-hexane (40 mg/mL). TEM analysis of the first solution (Figure 1a) confirmed the presence of nanoparticles of a variety of sizes, with diameters ranging from 5–7 nm. In the second synthesis, the amount of oleic acid was increased to 0.29 g (1.0 mmol), 15 mL of octyl ether was used in place of 1-octadecene, and the particles were precipitated with anhydrous isopropanol rather than ethanol. TEM analysis of the second solution (Figure 1b) again confirmed the presence of nanoparticles, but of a more monodisperse diameter distribution centered around 3 nm. The synthesis, workup and storage of the colloidal nanoparticle solutions was conducted in a helium atmosphere, so the nanoparticles were only exposed to air during the preparation of catalyst films.



Substrate Preparation

The FeMo nanoparticle catalysts were deposited onto conducting metal substrates by spin-coating at 2000 rpm unless otherwise noted. Inconel® 600 (Goodfellow) and Inconel® 625 (Arnold Magnetic Technologies) were cleaned with isopropanol and acetone and cut into 1.5 cm x 1.5 cm squares. Several of the substrates were first coated with alumina (~30 nm) by RF sputtering with an Al_2O_3 target (Cerac, 99.99%), followed by catalyst deposition. The amount of catalyst deposited onto the substrates was controlled by varying the volume of the FeMo nanoparticle solution

(40 mg/mL in hexane) used during spin-coating; in a standard synthesis, 0.25 mL of 5–7 nm catalyst particles were deposited onto an Inconel® 625 foil. The catalyst-coated substrates were allowed to dry in air and were then subjected to chemical vapor deposition to achieve CNT growth.

CNT Growth by CVD

Carbon nanotubes were synthesized by water-assisted chemical vapor deposition (CVD) as in [11] using a custom-built CVD system. Helium and hydrogen were used as the carrier gas with ethylene (all gases ultra-high purity) as the carbon source, and the flow rates were controlled by three mass flow controllers (MKS). After passing through its mass flow controller, the helium line was split and a small portion of the gas was humidified by passing it through a water bubbler. The gases were mixed and passed through a hygrometer (Shaw SD-G) before entering a 50-mm quartz tube furnace (18 inch long heating zone, Lindberg Blue-M). See Figure 2 for the layout of the CVD system. In a standard synthesis, up to four substrates were placed on a quartz boat in the center of the tube and heated to 750 °C under helium flow (540 sccm) over a ramp period of 20 minutes at a pressure of 760 torr. After reaching 750 °C, water bubbling was initiated, followed by addition of hydrogen (360 sccm) and ethylene (100 sccm). The water concentration ranged from 20–400 ppm and was typically maintained at 175 ppm, with a growth time of 10 minutes. These specific growth parameters were used as a standard and were systematically altered in different runs in an attempt to maximize the CNT growth yield and optimize the purity of CNTs obtained. At the end of the allotted growth time the hydrogen, ethylene and water sources were closed, and the samples were allowed to cool to room temperature under helium flow, at which time they were exposed to ambient atmosphere and subjected to various tests. The CNT growth yield was determined by subtracting the initial mass of the substrate and catalyst from the mass of the entire sample following the deposition and dividing by the area of the substrate.



Figure 2. Photograph of the custom-built chemical vapor deposition system.

Raman Spectroscopy

Raman spectroscopy was performed using the 2.33 eV (532 nm) line of an Nd:YAG laser. The back-scattered light was analyzed with a Jobin Yvon 270M spectrometer equipped with a liquid nitrogen cooled Spectrum One CCD and a holographic notch filter. A Nikon 55 mm camera lens was employed both to focus the beam on the sample and to collect the scattered light. Averaging three 30 second scans was sufficient to obtain high resolution Raman spectra.

BET Surface Area and Hydrogen Adsorption Measurements

The surface area of the CNTs was measured using a Quantachrome® Autosorb gas sorption system using nitrogen gas at 77K and utilizing the BET method to calculate the surface area. CNTs were removed from the conducting substrate using a razor blade, supported inside a platinum foil packet, and weighed on a microbalance. The initial BET measurement was carried out without degassing the CNTs, while two subsequent measurements were conducted after degassing the CNTs under vacuum at 200 °C and 350 °C, respectively.

The hydrogen adsorption was measured using a custom-built Sieverts apparatus, which consists of a known loop volume and an unknown sample tube volume separated by a valve. The loop was first pressurized to 3 400 torr with helium, which was allowed to expand into the sample tube at room temperature, where the pressure was monitored. Assuming that helium does not bind to the surface of the CNT sample, the pressure change can be used to calculate the volume of the sample in the tube using the Ideal Gas Law. The same procedure was then repeated with hydrogen in place of helium. The difference in pressure between the two gases corresponded to the amount of hydrogen adsorbed onto the CNT sample. The sample was then cooled to 77K with liquid nitrogen, and both the hydrogen and helium measurements were repeated to determine the cryogenic hydrogen storage capacity of the sample. As with the BET analysis, the first measurement was conducted without degassing the CNT sample, while two subsequent measurements were conducted after degassing the sample under vacuum at 200 °C and 350 °C, respectively.

Electrochemistry

Cyclic voltammetry was performed in a three-electrode cell with a platinum foil counter electrode, saturated Ag/AgCl reference electrode, and 1M H₂SO₄ electrolyte. The full CNT/FeMo/Inconel® electrode was connected to a copper wire using conductive copper tape, and a two component epoxy (LOCTITE 9462, Hysol) was used to shield the copper from the solution. The FeMo/Inconel® electrode was connected using a steel alligator clip. Scans were carried out at 100 mV/s after bubbling nitrogen through the solution for ten minutes, and the scans were repeated five times in order to allow for equilibration of the electrodes.

RESULTS

CNT Growth and Characterization

Visual analysis of the catalyst-coated substrates after chemical vapor deposition clearly indicated the presence of a relatively large amount of black, carbonaceous material (Figure 3). These deposits typically consisted of a thin base layer that was tightly bound to the substrate and very uniform in thickness and appearance, with

a thicker, more loosely bound, fluffy layer on top. Deposition was achieved under each growth condition tested as long as catalyst particles had been deposited on the substrates. Growth was also observed on the substrates which had undergone alumina sputtering, although the carbon material was much less tightly bound than on the plain Inconel® substrates and thus easily flaked off. A variety of different gas flow rates, growth times, humidity levels and catalyst concentrations were tested in an attempt to optimize the growth yield; these results are summarized in Figure 4 in terms of the deviation from the standard conditions presented above.

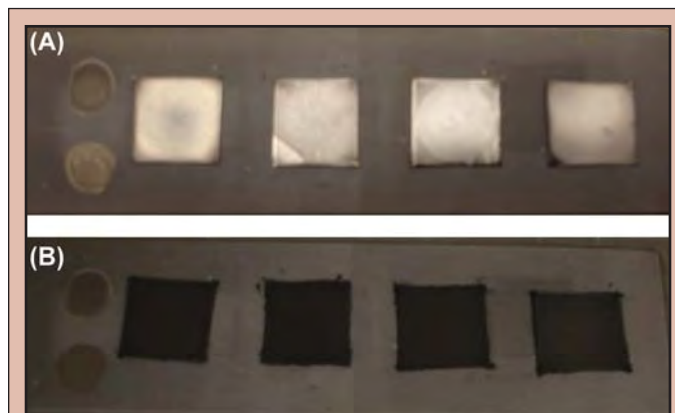


Figure 3. Photographs of FeMo-coated Inconel® substrates (A) before and (B) after chemical vapor deposition (utilized standard growth conditions as described in Materials and Methods section), clearly indicating the growth of carbon-containing materials.

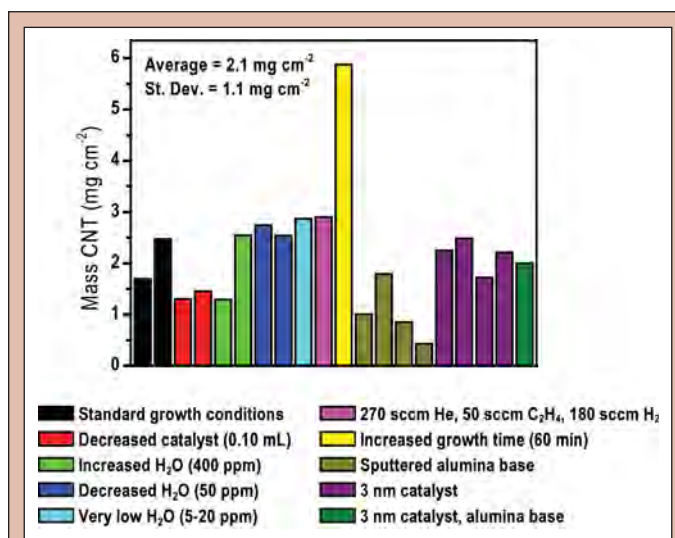
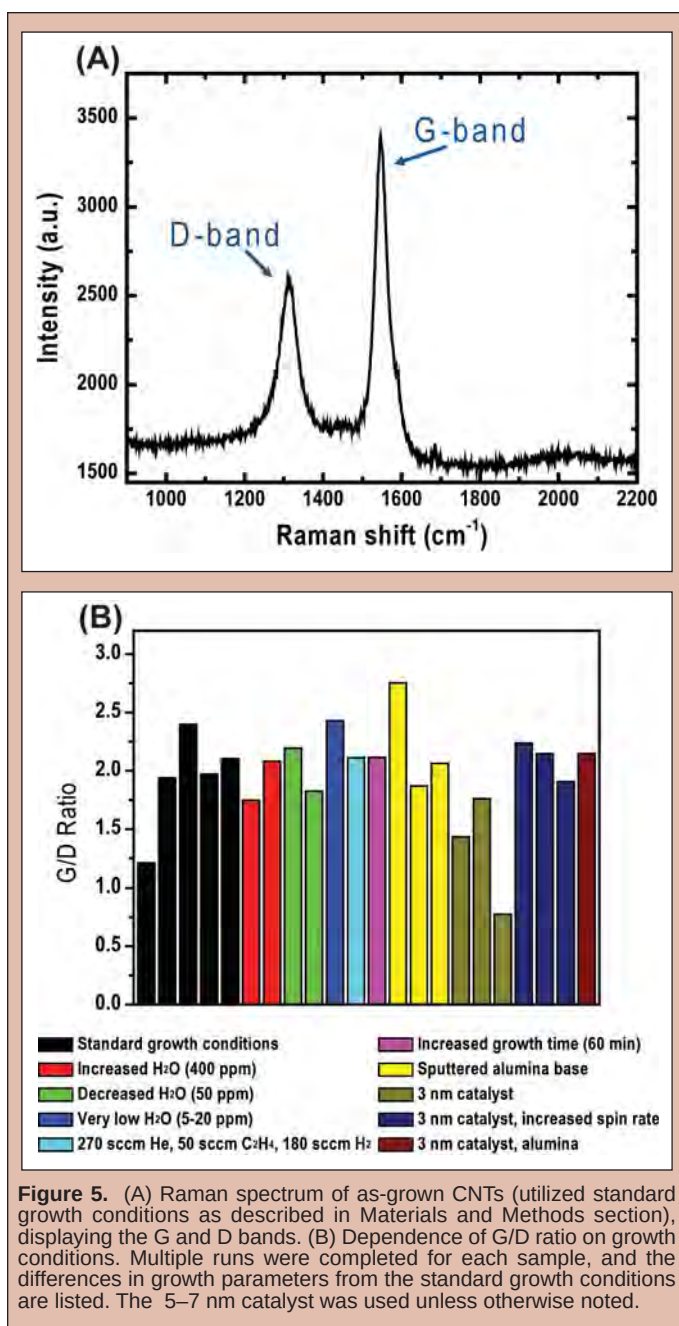
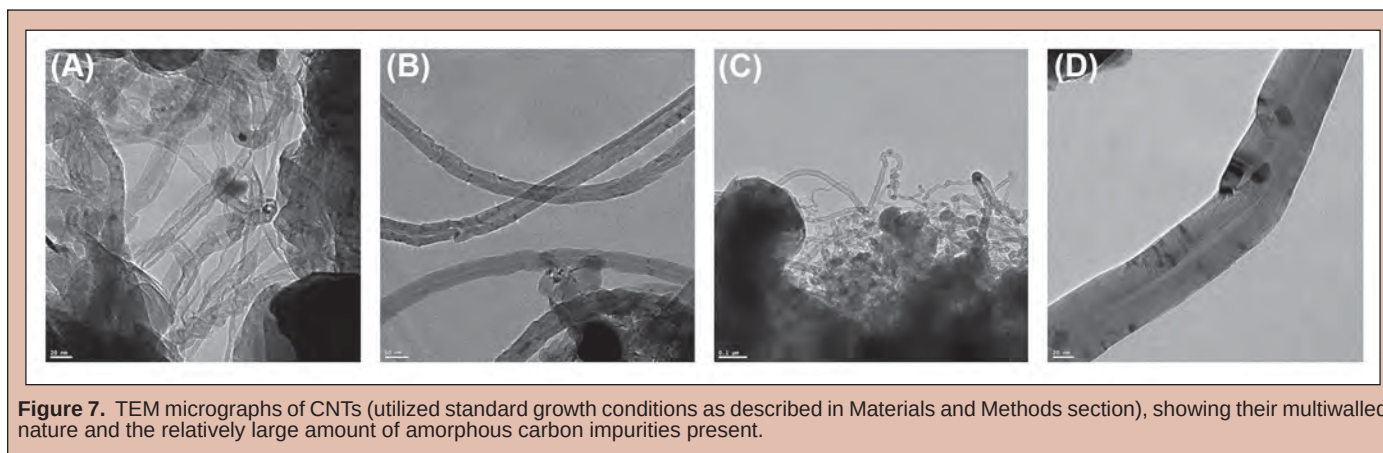
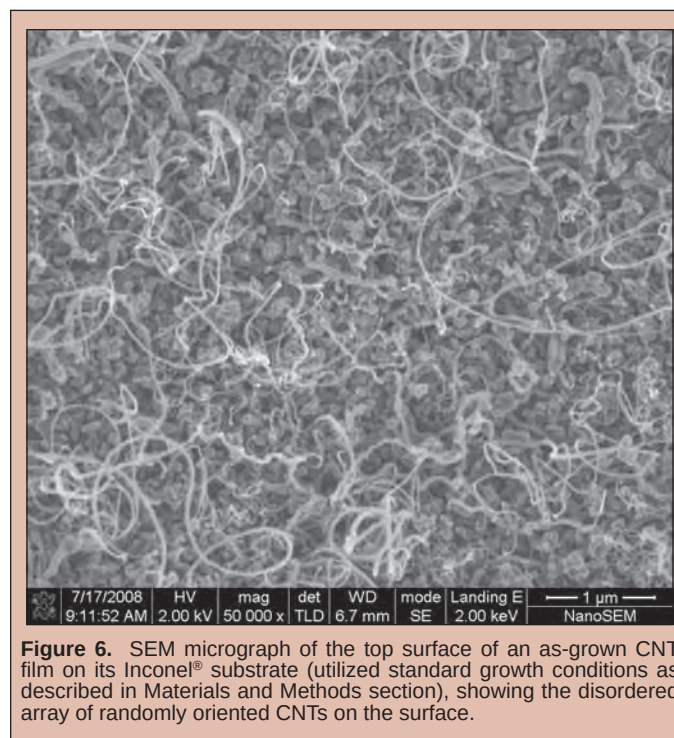


Figure 4. Dependence of CNT yield on growth conditions. Multiple runs were completed for each sample, and the differences in growth parameters from the standard growth conditions are listed. The 5–7 nm catalyst was used unless otherwise noted.

Raman spectroscopy provides a quick method for qualitatively assessing the purity of a sample of CNTs [32]. A broad peak occurring between ~1 300–1 400 cm⁻¹, which has been labeled the D-band, corresponds to amorphous carbon, metal catalyst particles and other impurities. A sharper peak at ~1 600 cm⁻¹, known as the G-band, corresponds to tangential vibration modes of carbon nanotubes. Thus, by comparing the intensity of the G-band to



that of the D-band in a specific sample, the relative amount of carbon nanotubes can be assessed. Raman spectra were collected and the G/D ratio was calculated for samples deposited under a variety of different growth parameters, with a characteristic Raman spectrum given in Figure 5a. The dependence of the G/D ratio on these parameter changes is summarized in Figure 5b. SEM and TEM images of the carbon materials were also collected. Characteristic SEM and TEM micrographs are given in Figures 6 and 7, respectively.



Energy Storage Investigations

The surface area and hydrogen adsorption of the carbon materials following different degassing temperatures, as measured by BET and Sieverts, respectively, are summarized in Table 1. The highest measured surface area was obtained after degassing the sample at 350 °C, with a value of 232 m²/g. The highest level of hydrogen adsorption was also achieved following the 350 °C degas, with a maximum of 0.85 wt%. Cyclic voltammetry scans of a FeMo/Inconel[®] electrode and a CNT/FeMo/Inconel[®] electrode are compared in Figure 8.

Degas	BET surface area	Cryogenic (77K) H ₂ adsorption
None	172 m ² /g	0.57 wt%
200 °C	223 m ² /g	0.41 wt%
350 °C	232 m ² /g	0.85 wt%

Table 1. BET surface area and cryogenic hydrogen adsorption of one CNT sample (utilized standard growth conditions as described in Materials and Methods section) following degassing at different temperatures.

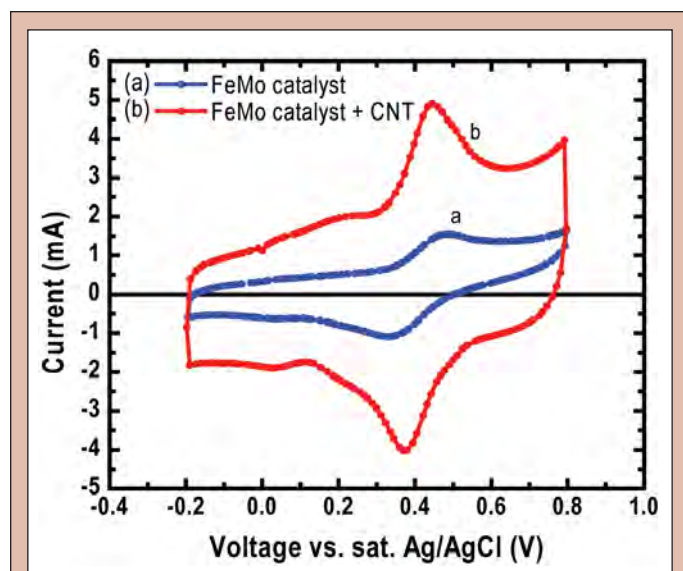


Figure 8. Cyclic voltammetry scan of (a) FeMo/Inconel[®] and (b) CNT/FeMo/Inconel[®] (utilized standard growth conditions as described in Materials and Methods section). The higher current displayed by (b) throughout the entire scan indicates capacitive charging of the electrode.

CONCLUSION

SEM and TEM analyses of the carbon materials clearly indicate that CNTs were, in fact, formed, but vertically-aligned growth was unverifiable. The large diameter (20–50 nm) and thick walls of the CNTs, as evidenced by TEM, suggest a multi-walled structure. CNTs appear to make up a minority of the sample and are only visible around the edges of large clusters of amorphous carbon. These microscopy findings are reinforced by Raman spectroscopy of the CNTs. The G/D ratio was fairly consistent across samples grown under different conditions, with an average intensity ratio of 1.96±0.42. While the greater size of the G-band does indicate the presence of CNTs, the low G/D ratio seen across all of the samples is suggestive of high amounts of amorphous carbon and

other impurities, in keeping with the SEM and TEM analyses. No discernable trend was extracted from the variation of the G/D ratio with growth conditions. The dependence of CNT yield on growth conditions is also fairly consistent (Figure 4), and a few trends are notable. First, under otherwise identical conditions, deposition of 0.25 mL of catalyst results in a higher yield than deposition of 0.10 mL of catalyst, with a negligible effect on the G/D ratio. Thus, increasing the catalyst concentration appears to simply result in a greater catalyst density and corresponding CNT density, rather than causing aggregation of the catalyst particles and a decrease in CNT selectivity. Secondly, increasing the growth time to 60 minutes from the usual 10 minutes brought about a roughly two-fold increase in growth yield without affecting the G/D ratio, indicating that the activity of the catalyst particles is considerably longer-lived than the 10 minutes used in most syntheses.

The measured BET surface area, which is 232 m²/g for these CNTs, is much lower than the ~1200 m²/g expected for single-walled CNTs, which should be expected given the large amounts of amorphous carbon and multi-walled CNTs in these samples. Despite this low surface area, however, these CNTs adsorb roughly 0.85 wt% of hydrogen, a relatively large amount. The Chahine rule predicts that for the physisorption of hydrogen onto carbonaceous materials, each 500 m²/g of surface area should result in 1 wt% of hydrogen storage [33]. Our CNTs thus appear to absorb ~80% more hydrogen than expected for typical carbon materials. One possible explanation for this high adsorption is hydrogen dissociation on FeMo catalyst particles that may still be present on the CNTs, allowing for spillover of hydrogen atoms into smaller, normally inaccessible pores. However, given the small sample size and large uncertainty in the measurement, more research into these materials is needed in order to confirm and determine the mechanism of increased hydrogen adsorption.

Cyclic voltammetry indicates the presence of two distinct electronic effects in the FeMo/Inconel[®] and CNT/FeMo/Inconel[®] samples (Figure 8). The FeMo/Inconel[®] scan is dominated by the reversible oxidation and reduction (redox) of the FeMo nanoparticles, most likely iron or iron oxide (no redox activity was observed for bare Inconel[®] substrates), with a small capacitive current present. The redox peaks are more pronounced in the CNT/FeMo/Inconel[®] sample but not significantly shifted in voltage, and there is also a much larger capacitive current throughout the whole voltage sweep as a result of capacitive charging of the CNTs. The CNT/FeMo/Inconel[®] sample thus displays both traditional capacitive charging as well as pseudocapacitive charging in the form of redox reactions of the FeMo nanoparticles. The specific capacitances of the FeMo/Inconel[®] sample and CNT/FeMo/Inconel[®] sample were calculated to be 2.0 F/g and 3.2 F/g, respectively, indicating a ~60% increase in capacitance upon introduction of CNTs. Our results demonstrate that water-assisted CVD is a promising method for producing CNTs, and identifies these CNTs as promising substrates for both hydrogen adsorption and supercapacitor electrodes.

Future Work

Additional work is needed to tune the CVD growth conditions in order to obtain higher-purity CNTs with less amorphous carbon, and to demonstrate vertically-aligned growth. One strategy is to use sputtered iron films rather than colloidal nanoparticles, which would

result in smaller catalyst particles and correspondingly thinner and more tightly packed tubes. More research is also needed to confirm and determine the reason for increased hydrogen storage in these CNTs and to determine if this level of storage can be optimized by increasing the specific surface area of the CNTs. These CNTs should also be investigated as support networks for hydrogen dissociation catalysts, and as conductive substrates for the deposition of redox-active transition metal oxides in supercapacitor applications.

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ADVANCES IN DUST DETECTION AND REMOVAL FOR TOKAMAKS

ALEJANDRO CAMPOS AND CHARLES H. SKINNER

ABSTRACT

Dust diagnostics and removal techniques are vital for the safe operation of next step fusion devices such as ITER. In the tokamak environment, large particles or fibers can fall on the electrostatic detector potentially causing a permanent short. An electrostatic dust detector developed in the laboratory is being applied to the National Spherical Torus Experiment (NSTX). We report on the development of a gas puff system that uses helium to clear such particles from the detector. Experiments at atmospheric pressure with varying nozzle designs, backing pressures, puff durations and exit flow orientations have given an optimal configuration that effectively removes particles from a 25 cm² area. Similar removal efficiencies were observed under a vacuum base pressure of 1 mTorr. Dust removal from next step tokamaks will be required to meet regulatory dust limits. A tri-polar grid of fine interdigitated traces has been designed that generates an electrostatic traveling wave for conveying dust particles to a "drain." First trials with only two working electrodes have shown particle motion in optical microscope images.

INTRODUCTION

Nuclear fusion is a promising alternative source of energy facing scientific and technical challenges. One of these challenges is the detection and removal of dust inside fusion reactors. Dust production results from the disassembly of plasma-facing tile surfaces or of co-deposited layers under intense transient heating by edge localized modes (ELMs) or disruptions. Dust can also appear as a result of the chemical agglomeration of sputtered C_n clusters [1]. Next step fusion devices, such as ITER, will produce larger quantities of dust, which could be radioactive from tritium or activated metals, toxic, and/or chemically reactive with steam or air [1]. The dust safety assessment value for ITER, which is the value above which the reactor's operation is unsafe, is 1000 kg. However, due to accounting uncertainties, the largest quantity of dust allowed in the reactor, also known as the dust administrative limit, is 670 kg. The amount of hot dust inside a reactor has lower limits. The limits for hot dust are 6 kg each for beryllium, carbon and tungsten. However, when there is no carbon dust inside the reactor, the limits are 11 kg for beryllium and 77 kg for tungsten [2]. Dust detection and removal techniques, which are still in their infancy, are vital to the safe operation of fusion reactors.

An electrostatic dust detector has already been developed and tested [3]. This detector consists of a grid of interlocking circuit traces, which are biased to voltages ranging from 30 V to 50 V.

Figure 1 shows a schematic of this device. A dust particle that falls on the detector causes a temporary short circuit, creating a voltage pulse recorded by standard nuclear counting electronics. The number of pulses is proportionally related to the mass of incident dust on the detector. The dust particles on the surface of the grid are usually vaporized or ejected from the detector, which restores the open circuit. However, some large particles or fibers stay on the surface and cause a permanent short circuit, which prevents the creation of further voltage pulses and impedes dust detection.

We have developed a gas puff system that blows helium gas on the surface of the detector to remove dust particles or fibers. A schematic of the gas puff system is shown in Figure 2. The system consists of a helium tank, a regulator, a shut-off valve that prevents or allows the flow of helium, a pressure meter that measures the gas pressure, a piezoelectric valve that controls the gas flow, and a nozzle through which helium is expelled. The piezoelectric valve is opened by a voltage pulse created by a pulse generator. This voltage pulse is monitored by an oscilloscope and is amplified by a driver. Gas is puffed in an inclined manner — the nozzle exit channel's longitudinal axis makes a 45° angle with the surface of the detector. This channel's diameter is 0.34 mm. The volume between the shut off valve and nozzle is 40.8 cm³ and the volume between the shut off valve and piezoelectric valve is 31.0 cm³. Our objective was to find the optimal gas puff system configuration that maximized the area of dust removed from the surface of the detector.

While the gas puff system clears dust from the surface of the electrostatic dust detector; the particles that are puffed away and other dust particles are deposited randomly on other areas inside the fusion reactor. Hence, another system is required to remove dust from the reactor itself. For this purpose, an innovative electrostatic dust transporter system that was recently designed and fabricated was tested.

Figure 3 shows a schematic of the electrostatic dust transporter system. The power supply generates three voltages, namely $+V/2$, ground and $-V/2$, which are transmitted to a triple rotary switch. This component sequentially switches the three voltages between the three electrodes of a tri-polar grid. The grid's electrodes branch out into fine interdigitated traces as shown in Figure 3. The resulting potential gradient on the surface of the tri-polar grid travels in a certain direction as the triple rotary switch sequentially switches



Figure 1. Schematic of the electrostatic dust detector is not drawn to scale. Particles falling in between the traces cause a temporary short circuit, which creates a voltage pulse that is recorded and related to the mass of incident dust.

the voltages. The potential gradient is repeated every three traces, resulting in a traveling electrostatic wave. A schematic of this wave is shown in Figure 4. Our objective was to test this system to observe particle motion and check the system's viability for dust removal. A more ambitious goal was to achieve consistent particle motion in one direction.

MATERIALS AND METHODS

Gas Puff System

A variety of short experiments was performed with the gas puff system to first investigate its properties and functioning. The highest voltage produced by the driver (corresponding to 20 half turns of the driver's control knob) best opened the piezoelectric valve. Nevertheless, this voltage was unknown since it was higher than the maximum value detected by the only available oscilloscope. The purpose of our first experiment was to predict the value of this high voltage. We measured different driver's output voltages detectable

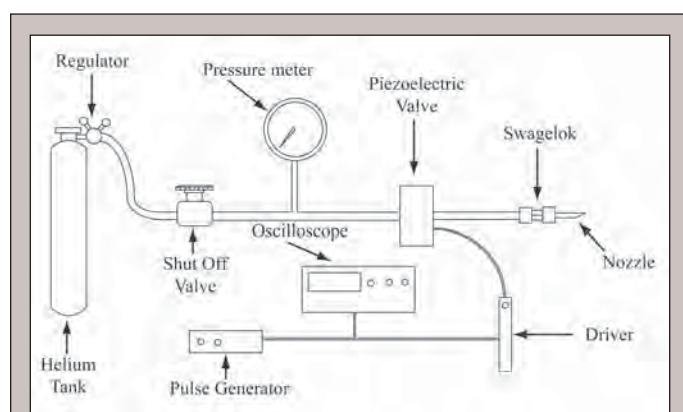


Figure 2. Schematic of the gas puff system, not to scale. Helium gas was blown through the system and was expelled at a 45° angle through the nozzle.

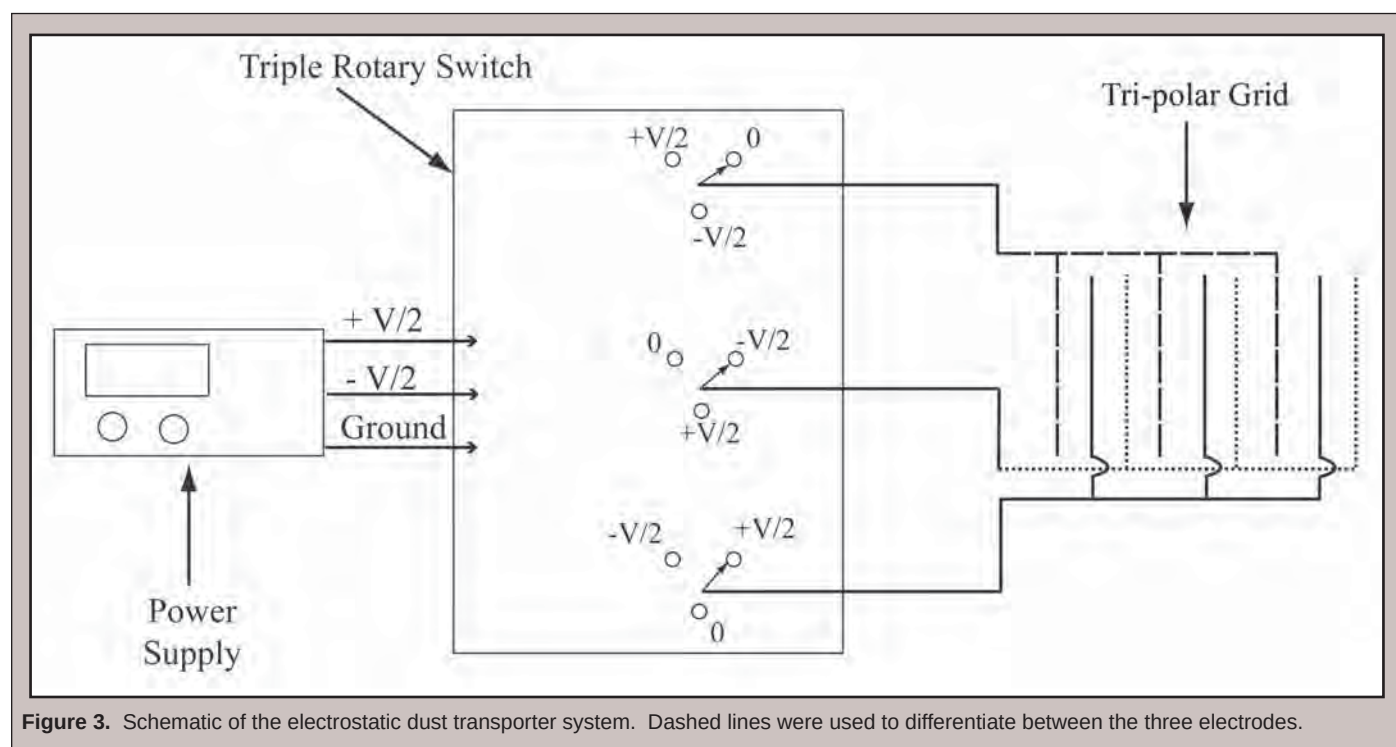
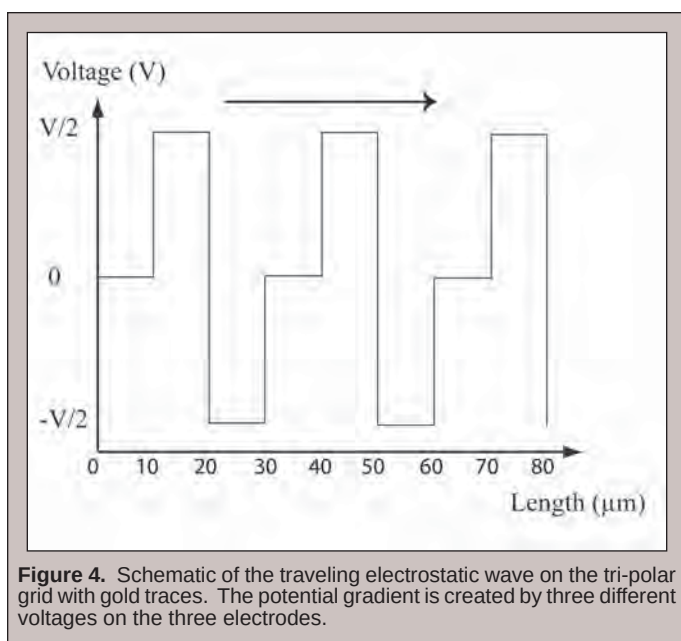


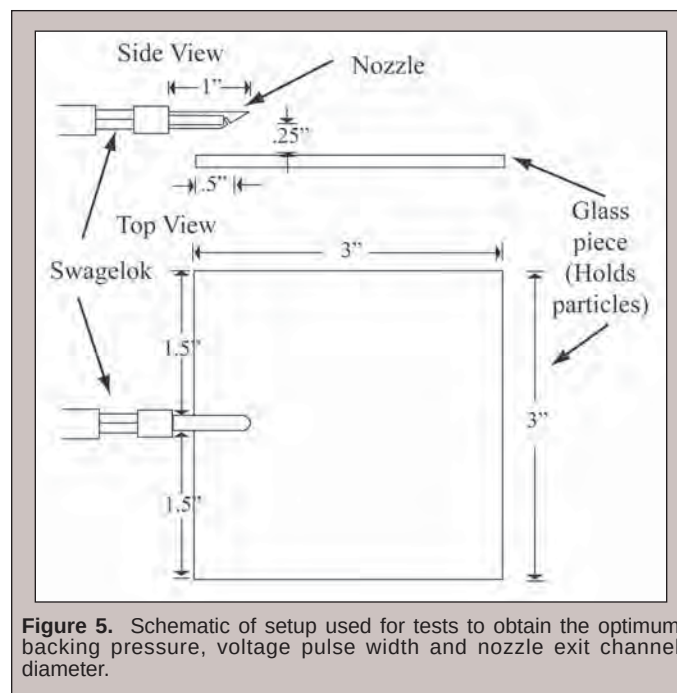
Figure 3. Schematic of the electrostatic dust transporter system. Dashed lines were used to differentiate between the three electrodes.



by the oscilloscope that corresponded to a number of half turns of the driver's control knob. A linear fit to the data was then obtained. The equation for this linear fit was used to predict the maximum voltage corresponding to 20 half turns of the control knob. The next short experiment consisted of measuring backing pressure as a function of the number of pulses provided to the piezoelectric valve. The initial backing pressure used was 40 psi, which was the maximum allowed by the initially available regulator. Equal pulses were continuously created to open the piezoelectric valve, and pressure was recorded after each pulse. We also measured pressure drop vs. backing pressure. Equal pulses were created at different backing pressures and the pressure drop was recorded after each pulse. Finally, we related pressure drop to voltage pulse width. First, a pulse with a specific length was created and the pressure drop was recorded. The backing pressure was then returned to its initial value of 100 psi, allowed by a new regulator. Finally, the process was repeated multiple times with varying pulse lengths.

After understanding the general characteristics of the gas puff system, tests were performed to find the most effective backing pressure, voltage pulse duration, and nozzle exit channel diameter and inclination. Tests were performed with sand placed on the surface of a 7.62 cm x 7.62 cm (3"x3") glass piece, at atmospheric pressure. To obtain the most effective backing pressure we first puffed helium to remove sand particles at different backing pressures. We then compared the resulting cleaned areas by observing pictures taken before and after puffing by a digital microscope. The backing pressures used were 40 psi, 60 psi, 80 psi and 100 psi. A schematic of the setup and nozzle location is shown in Figure 5. The same apparatus setup was used to obtain the optimal voltage pulse duration. We puffed helium to the surface of the glass containing sand particles using 250 ms, 500 ms, 750 ms and 1000 ms pulse durations. We then compared the pictures taken with the digital microscope of the glass before and after the puff. To obtain the most effective nozzle exit channel diameter, we puffed gas on the sand particles with nozzles of different diameter. We compared the area cleaned by each nozzle by observing the pictures taken with

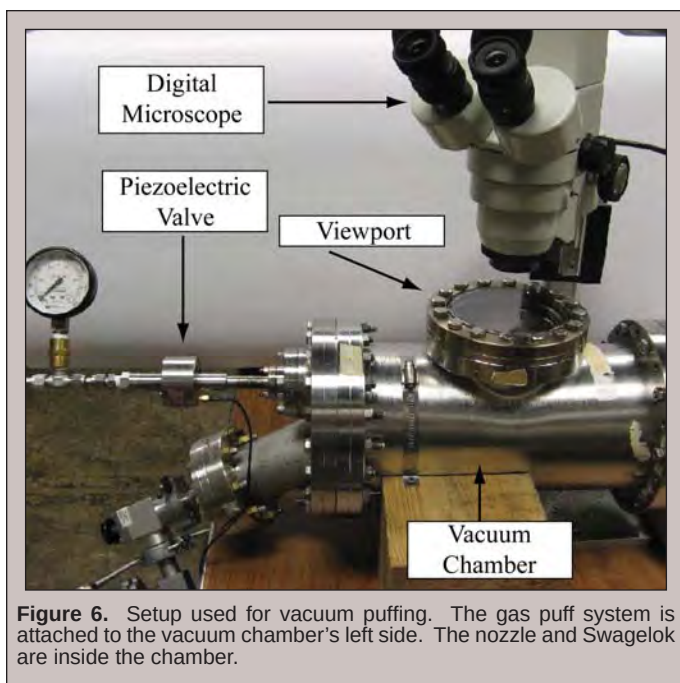
the digital microscope. Finally, to obtain the most effective nozzle exit channel inclination, we used different nozzle orientations to puff on the sand particles and compared the pictures taken with the digital microscope.



From the tests previously performed we obtained an optimal configuration that we used to puff sand particles, glass beads, carbon fiber composite (CFC) powder and tungsten particles at atmospheric pressure. Pictures were taken before and after the puff with both a digital microscope and a digital camera. Pictures taken with the camera provided a larger spatial coverage. After these tests were performed, puffing was done in a vacuum to simulate the dust environment. The nozzle and Swagelok were positioned inside a vacuum chamber, as shown in Figure 6. Sand, glass beads, CFC powder and tungsten particles were positioned on top of the 7.62 cm x 7.62 cm (3"x3") glass piece, which in turn was positioned on top of a tray inside the chamber. The base pressure for vacuum puffing was 1 mTorr. Pictures were again taken with a digital microscope and a digital camera, which showed the particles through a viewport on the upper side of the chamber. This setup is shown in Figure 6.

Electrostatic Dust Transporter System

Two types of tri-polar grid devices were tested. One consisted of chromium electrodes 25 μm thick and 25 μm apart; the other consisted of gold electrodes 10 μm thick and 10 μm apart. The electrodes are insulated with a 300 nm thick silicon nitride (SiN_x) layer. The grid devices were fabricated by the Princeton Microelectronics Group using standard photolithography techniques. Carbon and tungsten particles were positioned on top of the tri-polar grid. Pictures of the particles on the grid were taken with a high resolution digital microscope before and after the electrodes were charged, and before and after every voltage switch caused by the triple rotary switch. The pictures obtained were later compared to observe any particle motion. Voltage switches with the triple rotary switch were manually performed every few seconds.

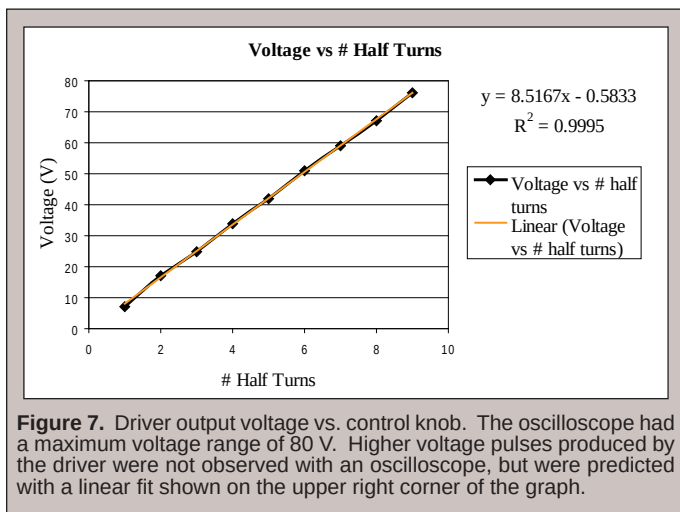


Moreover, all tests were performed with grids that contained only two working electrodes, since fully functional grids were unavailable. Grids with two working electrodes produce a traveling electrostatic wave whose profile is different for each voltage switch. Nevertheless, potential gradients are still generated, which are responsible for particle motion.

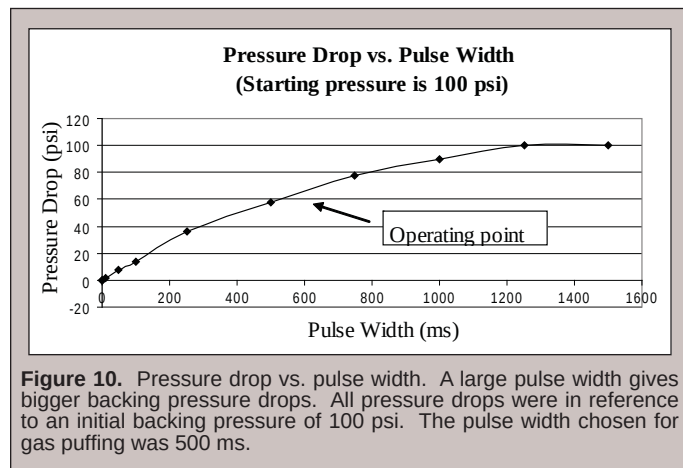
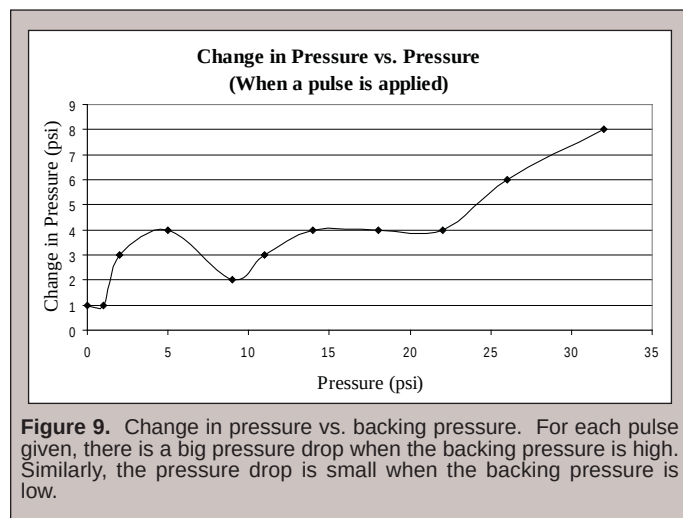
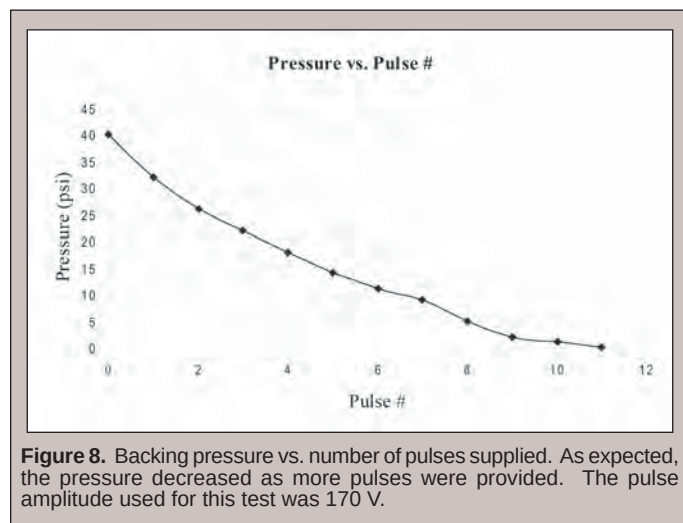
RESULTS

Gas Puff System

The first short experiments provided useful information regarding the properties and functioning of the system. The linear fit to the data points representing voltages given by the number of the control knob's half turns represented the data accurately. Thus, high confidence was placed on the accuracy of the predicted maximum voltage. This linear fit gave a maximum voltage of 170 V for 20 half turns of the control knob. The data points are shown in Figure 7. Also, backing pressure decreased as the number of pulses given increased, which showed correct functioning of our system and



agreed with our expectations. Data for this experiment is shown in Figure 8. Additionally, the pressure drop is higher at high backing pressures, and lower at low backing pressures, as observed in Figure 9. This experiment indicated puffs with high backing pressures emit larger gas quantities and are expected to remove more dust particles. Finally, longer pulse widths gave bigger pressure drops and vice versa, as expected. The results are shown in Figure 10.



Experiments performed to obtain the optimal configuration of the gas puff system yielded the following results. By observing pictures obtained with the microscope we concluded that higher backing pressures increased the area cleaned and that 100 psi was the most effective pressure allowed by our regulator. Moreover, longer pulse durations did not increase the cleaned areas, since most of the particles were removed within the first instances of the puff. Hence, to minimize the amount of gas wasted, a 500 ms pulse was chosen as the optimum, since it was as efficient as pulses with longer durations. Also, the nozzle with the smallest exit channel diameter, namely 0.34 mm, most effectively removed the particles. Finally, vertical puffing increased the area cleaned as opposed to horizontal puffing. However, space constraints limited puffing to an inclination of 45°. Thus, we decided to fabricate a nozzle with the maximum allowable exit channel inclination.

Both sand particles and glass beads were easily removed at atmospheric pressure with a puff, which created a 5 cm x 5 cm clean area. Carbon particles were also easily removed, giving a 4 cm x 4 cm clean area. Figure 11 shows pictures taken with the digital microscope and regular camera before and after puffing CFC powder at atmospheric pressures. Tungsten particles were harder to remove, since they adhered to the glass surface. The area cleaned for tungsten particles was around 3 cm x 3 cm at atmospheric pressure. Figure 12 shows pictures taken with the digital microscope and regular camera before and after puffing tungsten particles.

The cleaning effectiveness for vacuum puffing did not improve. Tungsten was again removed from a 3 cm x 3 cm area, carbon was cleaned from a 4 cm x 4 cm area, and sand and glass beads were removed from a 5 cm x 5 cm area. Figures 13, 14 and 15 show pictures of sand particles, CFC powder and tungsten particles in a vacuum, before and after the puff. Tungsten particles were dried by heating them in an oven for an hour, which minimizes moisture effects and makes them less adhesive to the glass piece. This process, however, did not improve the cleaning effectiveness.

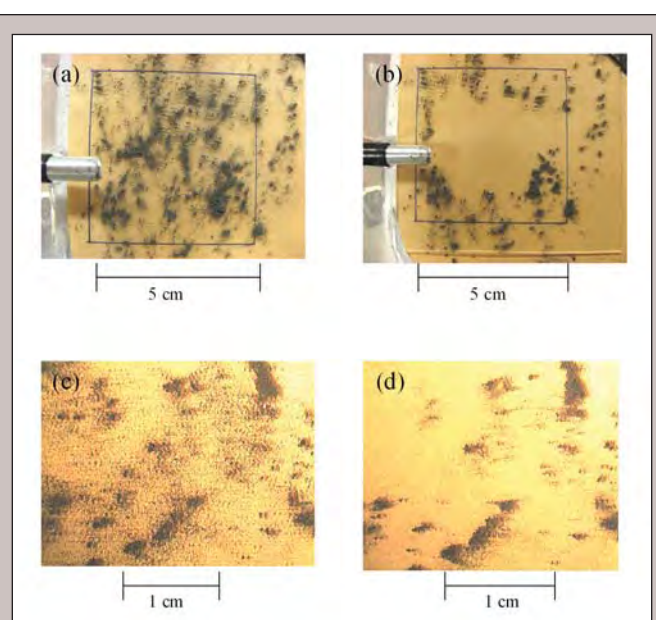


Figure 12. Pictures of tungsten particles at atmospheric pressure, taken (a) with digital camera before puff, (b) with digital camera after puff, (c) with digital microscope before puff and (d) with digital microscope after puff.

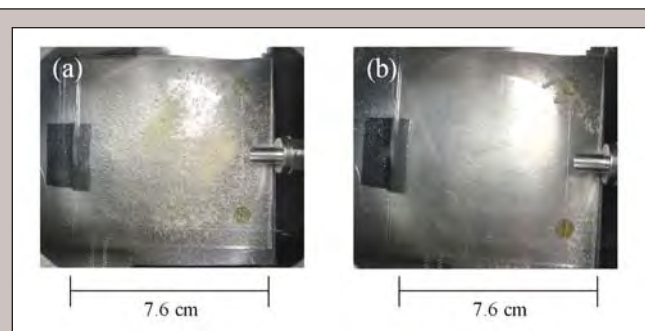


Figure 13. Pictures taken with digital camera of sand particles at base vacuum pressure of 1 mTorr (a) before and (b) after puffing.

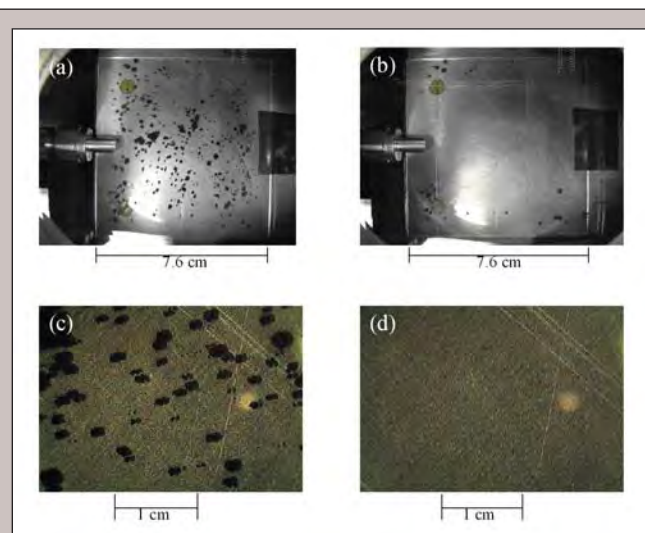


Figure 14. Pictures of carbon particles at base vacuum pressure of 1 mTorr taken (a) with digital camera before puff, (b) with digital camera after puff, (c) with digital microscope before puff and (d) with digital microscope after puff.

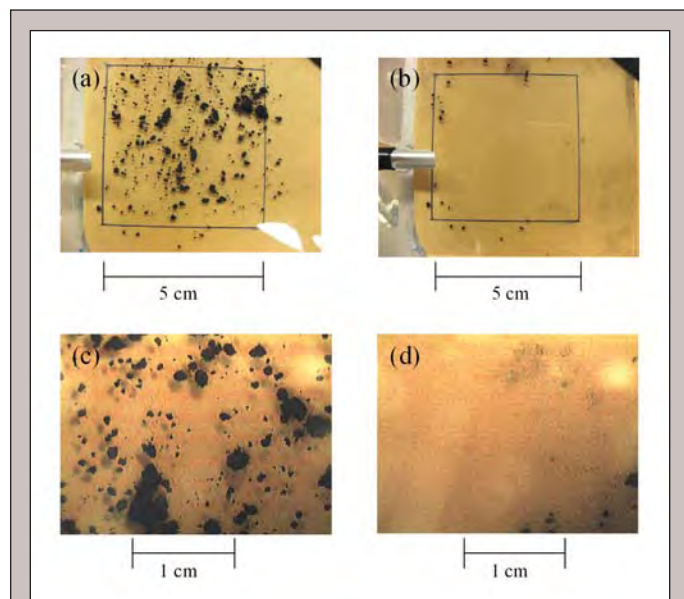
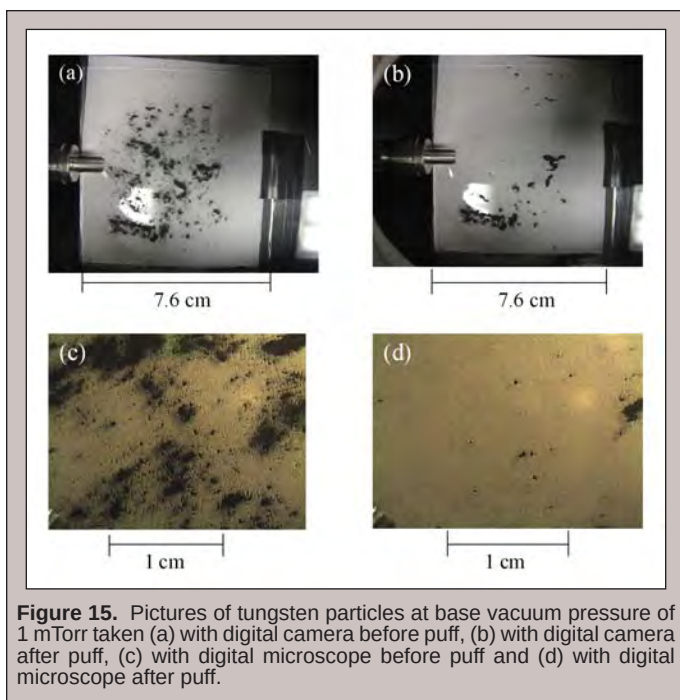
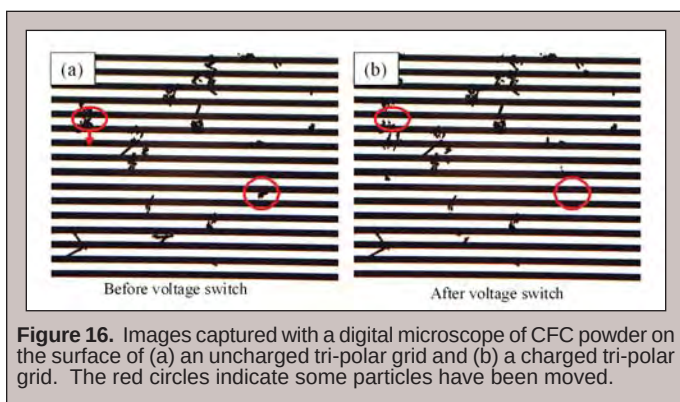


Figure 11. Pictures of carbon particles at atmospheric pressure taken (a) with digital camera before puff, (b) with digital camera after puff, (c) with digital microscope before puff and (d) with digital microscope after puff.



Electrostatic Dust Transporter System

The results from the tests performed show particle motion. 50 V, 0.0 V and -50 V were applied to the triple rotary switch. When the power was turned on, motion of some particles was observed. As the voltages were sequentially switched more particle motion was observed. However, after one or two switches, particle motion stopped. Figure 16 shows two pictures, one of carbon particles on top of an uncharged tri-polar grid, and the other of carbon particles after the power was turned on. The red circles show a particle's location before the tri-polar grid was charged. After the voltages were supplied, the particles were not located within those circles, as shown by the second picture in Figure 16.



DISCUSSION AND CONCLUSION

Gas Puff System

The biggest electrostatic dust detector fabricated has a surface area of 5 cm x 5 cm. Our gas puff system was able to clear off carbon particles from a 4 cm x 4 cm area, which is very close to the required area. Tungsten particles were removed from a 3 cm x 3 cm area, which is a good achievement, yet it is not a large enough area to cover

the entire surface of the detector. These results were achieved using the maximum allowed backing pressure. Therefore, tests should be performed to see if an increase of the exit flow momentum due to higher backing pressures increases cleaning effectiveness. Tests could be carried out with a gas puff system that has a regulator, pressure gauge and connecting tubes able to contain higher pressures. Additionally, tests should be conducted with a system containing two nozzles used to increase the emission of helium. This setup may be more effective at removing particles from the corners of the detector, where they are difficult to reach using our current system. Finally, simulations of the helium flow field on the surface of the glass piece could be performed with a computational fluid dynamics code, which may suggest better gas puff system designs.

Electrostatic Dust Transporter System

All research was conducted with grids that had only two functional electrodes. The tri-polar grids are very delicate since a light scratch easily damages an entire section or an electrode. More experience with their fabrication will make their manufacturing a faster process, and will also improve their quality and resistance. Despite using only two electrodes, the tri-polar grid produced some particle motion. This initial result suggests the electrostatic dust removal system is a feasible removal mechanism. As with the case of the gas puff system, further tests will be conducted in which a fully functional grid is used. Tests will be performed with this mechanism with the hope of obtaining unidirectional particle motion, which will better determine the ability of this system to transport dust particles.

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MASSIVELY PARALLEL LATENT SEMANTIC ANALYSES USING A GRAPHICS PROCESSING UNIT

JOSEPH CAVANAGH AND XIAOHUI CUI

ABSTRACT

Latent Semantic Analysis (LSA) aims to reduce the dimensions of large term-document datasets using Singular Value Decomposition. However, with the ever-expanding size of datasets, current implementations are not fast enough to quickly and easily compute the results on a standard PC. A graphics processing unit (GPU) can solve some highly parallel problems much faster than a traditional sequential processor or central processing unit (CPU). Thus, a deployable system using a GPU to speed up large-scale LSA processes would be a much more effective choice (in terms of cost/performance ratio) than using a PC cluster. Due to the GPU's application-specific architecture, harnessing the GPU's computational prowess for LSA is a great challenge. We presented a parallel LSA implementation on the GPU, using NVIDIA® Compute Unified Device Architecture and Compute Unified Basic Linear Algebra Subprograms software. The performance of this implementation is compared to traditional LSA implementation on a CPU using an optimized Basic Linear Algebra Subprograms library. After implementation, we discovered that the GPU version of the algorithm was twice as fast for large matrices (1000x1000 and above) that had dimensions not divisible by 16. For large matrices that did have dimensions divisible by 16, the GPU algorithm ran five to six times faster than the CPU version. The large variation is due to architectural benefits of the GPU for matrices divisible by 16. It should be noted that the overall speeds for the CPU version did not vary from relative normal when the matrix dimensions were divisible by 16. Further research is needed in order to produce a fully implementable version of LSA. With that in mind, the research we presented shows that the GPU is a viable option for increasing the speed of LSA, in terms of cost/performance ratio.

INTRODUCTION

Considering the large amount of data being collected annually, methods are needed to extract valuable information from this data [1]. Latent Semantic Analysis (LSA) is a numerical technique used to extract information from large collections of text documents such as relationships between various terms, sentences and full documents [2]–[3]. LSA works by taking the singular value decomposition (SVD) of $\mathbf{A}$ where $\mathbf{A} = \mathbf{D} \mathbf{D}^T$, with $\mathbf{D}$ being the term-document matrix. A term-document matrix contains a numerical value for each term in its respective document, with the documents representing the columns of the matrix and the terms representing the rows of the matrix. Since there are often 5 000 or more unique terms, and documents may contain only a couple hundred terms, many of the matrix values become zero. The term-document matrix is created beforehand, using a term weighting and text stripping algorithm such as a Term Frequency-Inverse Document Frequency (TF IDF) [14]. The core of the SVD algorithm requires an eigendecomposition of the matrix, which has been a computational problem for many

decades [2], [7]–[8], [11]. This makes SVD a computationally expensive algorithm, which makes it a prime candidate for decreasing processing times [2], [7], [11]. Many modern SVD methods tridiagonalize $\mathbf{A}$ before computing the SVD, due to the performance increase between calculating SVD on a normal matrix and a tridiagonal matrix [2], [7]–[8], [15]. A tridiagonal matrix is a matrix with values only in its main diagonal, one element above the main diagonal, and one element below the main diagonal. All other elements in the matrix are set to zero. Tridiagonalization takes up a large portion of the time for computing the SVD, so our main focus is our parallel algorithm which saves computation time.

Recently, the graphics processing unit (GPU) has become a focus for inexpensive, high performance computing in various scientific fields [10]. Due to the massively parallel architecture of the GPU, it is able to perform floating point calculations much faster than a standard central processing unit (CPU) [10]. We performed the CPU benchmarks on a Dell™ Precision 370 using SiSoftware® Sandra, a program for benchmarking various computer

components. When this paper was written, an Intel™ Pentium 4 3.6 GHz CPU was priced around \$140 and produced 11 gigaflops (one billion floating point operations per second). An NVIDIA® 1 GB 8800 GT GPU cost around \$200 and produced around 300 GFLOPS. The price-to-performance ratio for the CPU is 0.079 GFLOPS/dollar, while the GPU price-to-performance ratio is 1.5 GFLOPS/dollar. The impressive price-to-performance ratio of the GPU makes it a prime candidate for increasing the speed of LSA while still using components found in many desktop and laptop personal computers.

The increased performance of the GPU comes with certain difficulties. Memory transfer from system memory to GPU memory (host to device and device to host) remains relatively slow and can often be a bottleneck in many applications. Most current GPUs offer support for only single precision, while many scientific applications require double precision support. Also, certain algorithms are primarily serial, prohibiting much of the GPU's processing power from being utilized. For each of these problems a solution must be found. Currently, the effect of slow memory transfer can be minimized by performing as many GPU-based computations as possible between transfers. Transferring large amounts of data at one time is generally faster than making numerous small memory transfers. Double precision can be either emulated by an algorithm or can be obtained by purchasing a new NVIDIA® 200 series GPU.

Our literature research shows that there is currently no GPU-based implementation of LSA. Related research includes a team at the University of North Carolina at Chapel Hill that used a GPU-based algorithm for solving dense linear systems [4]. Their implementation of an LU decomposition algorithm performed 35% better than an Automatically Tuned Linear Algebra Subroutines (ATLAS) implementation on the CPU for matrices of rank 3500. Manavski and Valle have implemented the Smith-Waterman algorithm on the GPU [9]. The Smith-Waterman algorithm explores alignments between two sequences in protein and DNA databases. Their implementation ran between two and 30 times faster than other implementations for commodity hardware. Another example of the power of the GPU is given in the literature [13]. Robert, Schoepke and Bieri used the GPU to implement ray tracing algorithms and then compared the results to an implementation on a CPU. In an animated example, the GPU performed around six times better than the CPU. These examples show that the GPU is a powerful tool that, when used correctly, can be used to increase the speeds of a variety of algorithms in a variety of fields.

MATERIALS AND METHODS

For our implementation, we decided to use a Lanczos algorithm to assist with the SVD. The Lanczos algorithm tridiagonalizes a matrix which allows for the computation of SVD to be performed significantly faster [8]. This is done by using various matrix-vector and vector-vector operations in order to achieve a Krylov subspace. This subspace is a representation of the original matrix and maintains approximate eigenvalues and eigenvectors to that of the original matrix. The reason we chose Lanczos is that it is not as computationally demanding as alternative options. The algorithm can be seen in Figure 1. The vector *alpha* is then used to form the main diagonal of the new matrix, where the vector *beta* will form the subdiagonal and superdiagonal. This algorithm is proven to be

accurate in an environment without rounding errors. However, due to the fact that our GPU supports single precision, rounding errors are inevitable. Maintaining accuracy while using the GPU will be discussed more in the *Discussion and Conclusion* section.

```

Algorithm Lanczos
 $v_1 \leftarrow$  random vector with norm 1.
 $v_0 \leftarrow 0$ 
 $\beta_1 \leftarrow 0$ 
Iteration: for  $j = 1, 2, \dots, m$ 
     $w_j \leftarrow Av_j - \beta_j v_{j-1}$ 
     $\alpha_j \leftarrow (w_j, v_j)$ 
     $\tilde{w}_j \leftarrow w_j - \alpha_j v_j$ 
     $\beta_{j+1} \leftarrow \|\tilde{w}_j\|$ 
     $v_{j+1} \leftarrow \tilde{w}_j / \beta_{j+1}$ 
return

```

Figure 1. Lanczos Algorithm [8].

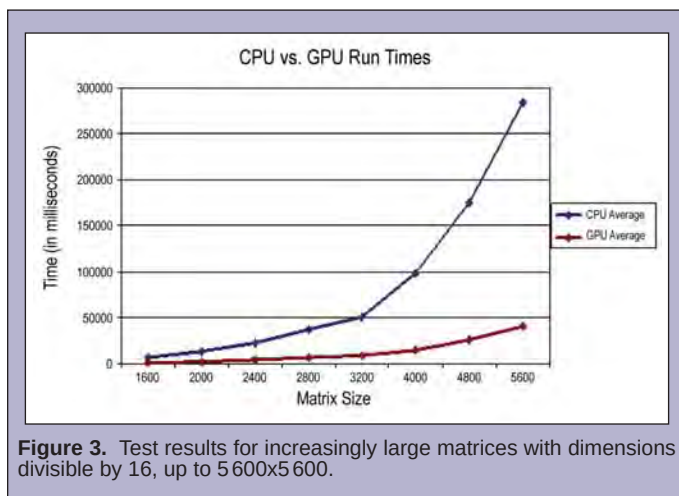
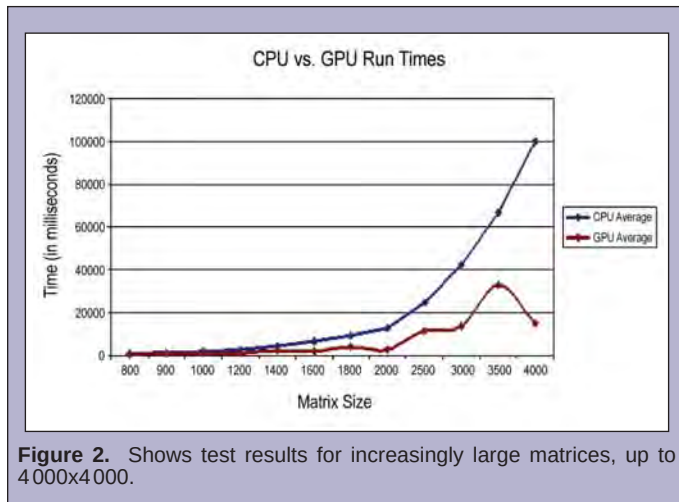
Our GPU implementation uses Compute Unified Basic Linear Algebra Subprograms (CUBLAS) to perform the matrix-vector and vector-vector operations that the algorithm requires. CUBLAS is a Compute Unified Device Architecture (CUDA) implementation of Basic Linear Algebra Subprograms (BLAS) which has been tuned to provide good performance across a variety of GPUs. To avoid bias, we compare our performance with the Intel® Math Kernel Library. The linear algebra routines from the BLAS libraries used in both the CPU and GPU implementations were identical. The only difference was that the algorithmic designs of each version were used in order to extract performance out of their respective architectures. The main linear algebra routines used are *sge mv*, *saxpy*, *sdot* and *snrm2*. These routines are frequently used for basic linear algebra functions that were developed to provide building blocks for larger applications. If $A = D \cdot D^T$, with D representing the term-document matrix, only A needs to be stored in memory on the GPU, along with a few vectors which are a fraction of the data size of D . This is very advantageous, as the memory on a GPU card can be a very limiting factor. The card used for our testing has 1 GB of memory, which allows us to allocate about 950 MB to use in our program. The extra memory which cannot be allocated is due to a process behind the scenes preventing full allocation. The CUDA community currently regards this as a bug as it is unclear why this much memory is reserved for other uses. With 950 MB of usable memory, we are able to allocate matrices that exceed 15 000x15 000. This is well within the matrix size targeted for our algorithm.

After implementing the CPU- and GPU-based algorithm, we timed each implementation for various matrix sizes. The computer testing the implementations has the following specifications: one 3.6 GHz Intel Pentium 4 CPU, 3.00 GB of RAM, NVIDIA® 8800 GT with 1 GB device memory, 160 GB hard drive. Three randomly generated matrix sizes were selected in an interval thought to clearly display the performance of each implementation, to perform the LSA of each matrix. For each of the three matrices, both CPU and GPU versions are run five times and the total time is averaged. This produces 15 total runs for both the CPU and

GPU at every matrix size interval. The times are then averaged for display purposes.

RESULTS

Our initial results can be seen in Figure 2, which is for matrices up to 4000x4000. These initial results show a performance increase of two to six times. Figure 3 shows the average CPU and GPU run times for matrices that have dimensions divisible by 16. The tests were performed in the same manner as the original tests, with the only change being the matrix sizes. The GPU in this scenario is able to process the data from four times faster (for a 1600x1600 matrix) up to almost seven times faster (for a 5600x5600 matrix).



The CPU version takes about twice as long for the majority of matrices 1000x1000 and larger. For matrices smaller than this, the speed increase is less noticeable. For extremely small matrices (smaller than 600x600) the CPU version is faster than the GPU version. The reasoning for this is that using the GPU requires significant constant overhead, which can consume a large percentage of the time [10]. When matrix sizes are increased, the percentage of the total time that the overhead consumes is decreased. This is because the overhead time does not change, but the amount of computation being done significantly increases. Even for matrices near the high end of our selected sizes, the GPU is nearly twice as fast.

DISCUSSION AND CONCLUSION

After testing our algorithm, it became evident which areas needed further research to produce an effective, fully implementable algorithm. The first area to be addressed is the accuracy of the algorithm. Currently, spurious eigenvalues and their resulting vectors are being created due to rounding errors. These are generated during the tridiagonalization process [8], [12], [15]. Two methods may be used in this situation. Either the spurious values can be removed after computation or reorthogonalization can be performed during computation [12], [15]. Removing spurious values after computation, while technically possible, is thought to be less effective than reorthogonalization. Reorthogonalization is the process of ensuring that the generated vectors are an accurate sub-space representation of the original matrix. For this reason, we will aim to implement partial reorthogonalization. Partial reorthogonalization has been proven to be able to preserve semiorthogonality [11], [15]. Partial reorthogonalization would allow us to stop our iteration sequence shorter than a simple Lanczos algorithm. These reasons make a partial reorthogonalization method necessary in a fully implementable LSA algorithm.

Another area of interest in future research would be further increases in the speed of the algorithm. Currently the GPU is only being used for the tridiagonalization computation. However, the *sstev* BLAS routine, which computes the eigenvalues and eigenvectors of a tridiagonal matrix, is still being implemented on the CPU. Transitioning this to the GPU should further increase the performance of the algorithm. The percentage of the total computation time that *sstev* occupies is only around 5% (for a 4000x4000 matrix). As matrix sizes grow, the total time that *sstev* requires will also grow, making a GPU version of the routine highly useful. This is especially true if the matrix sizes are approaching 10000x10000. Also, improvements upon the CUBLAS *sgemv* routine, which is a matrix-vector multiplication routine, would greatly increase performance as 90% of the GPU computation time is being occupied by this routine. This is entirely feasible as CUBLAS is not stated as being the optimal implementation.

A final area of research would be to attempt to implement the algorithm on a multiple GPU machine. Currently, in order to use multiple GPUs, the algorithm must explicitly state how to use the GPUs. There is no automatic optimization allowing the use of multiple GPUs. For this reason, code needs to be modified for each individual problem. The use of multiple GPUs would be highly beneficial due to the increase of raw computational power. Numerous computers are being released with multiple graphics cards built in or with the capability to add a second graphics card. Adding multi-GPU functionality can be tricky and does not always increase the speed of code because very little effective communication happens between GPUs. This makes sharing computation of problems very difficult, such as when computing a matrix-matrix product. In order to complete the computation, a GPU must have each matrix in its global memory. This adds a lot of increased overhead, as copying memory between GPUs currently requires copying from GPU 1 to the computer then from GPU 2 to the computer. This is very slow and limits the effectiveness of multi-GPU implementation. Further research would be needed to investigate multi-GPU capabilities.

The select few matrices that seem to be performing significantly better than average, specifically matrices with a rank of 2000, 3200 and 4000, are a result of the unique architecture of the GPU. These select few matrices all have one thing in common: The matrix dimensions are all divisible by 16. The reason behind the significant speed increase lies in the architecture of the GPU. When the matrix is not divisible by 16, there are conflicts in shared memory regarding multiple threads accessing the same bank at the same time. This forces one thread into a queue while the other thread is accessing the memory, increasing the total amount of time for all memory accesses. This can be solved by using matrices with dimensions divisible by 16. CUBLAS will as a result provide coalesced memory access patterns, greatly reducing time of the overall function. This was not evident until after obtaining the results, which led us to further test the implementations to verify problem with memory access patterns.

In this research, we developed a parallel latent semantic analysis algorithm for the GPU. The results of our tests are very promising. The speed increase of the GPU based algorithm was five to seven times for matrices with dimensions divisible by 16 and two times for matrices of other sizes. One solution to ensuring that all matrices have dimensions divisible by 16 is to add extra columns and rows of zeros to the matrix. The number of rows and columns to add would be equal to $(x \bmod 16)$ where x is equal to the dimension size of the matrix. This number would always be between 1 and 15, requiring minimal computation time when adding this data. We hypothesize that adding these rows and columns of zeros would not add a noticeable increase to computation time and thus would still yield a speed increase of five to seven times. With the GPU being so widespread in modern PCs, this algorithm is not just limited to expensive custom workstations. Most mid-range computers currently come with a graphics card, including laptops. This makes it possible to perform GPU-based LSA on a mobile computer. That being said, a top of the line desktop computer would be expected to see even better results. Currently, the NVIDIA® 280GTX has a theoretical computation level of about 1 teraflop. This is more than twice that of the card we used and costs approximately 115% more. With GPU computational power increasing at a higher rate than CPU computational power, it is very possible to see increased speed results in the near future [10]. We have shown that the GPU can be used to provide a performance increase to our algorithm. This should not only be useful to us, but it will provide evidence to further algorithmic development of the GPU.

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IMIDAZOLE-BASED IONIC LIQUIDS FOR USE IN POLYMER ELECTROLYTE MEMBRANE FUEL CELLS: EFFECT OF ELECTRON-WITHDRAWING AND ELECTRON-DONATING SUBSTITUENTS

ELIOT CHANG, YONGZHU FU AND JOHN KERR

ABSTRACT

Current polymer electrolyte membrane fuel cells (PEMFCs) require humidification for acceptable proton conductivity. Development of a novel polymer that is conductive without a water-based proton carrier is desirable for use in automobiles. Imidazole (Im) is a possible replacement for water as a proton solvent; Im can be tethered to the polymer structure by means of covalent bonds, thereby providing a solid state proton conducting membrane where the solvating groups do not leach out of the fuel cell. These covalent bonds can alter the electron availability of the Im molecule. This study investigates the effects of electron-withdrawing and electron-donating substituents on the conductivity of Im complexed with methanesulfonic acid (MSA) in the form of ionic liquids. Due to the changes in the electronegativity of nitrogen, it is expected that 2-phenylimidazole (2-PhIm, electron-withdrawing) will exhibit increased conductivity compared to Im, while 2-methylimidazole (2-MeIm, electron-donating) will exhibit decreased conductivity. Three sets of ionic liquids were prepared at defined molar ratios: Im-MSA, 2-PhIm-MSA, and 2-MeIm-MSA. Differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and ^1H -NMR were used to characterize each complex. Impedance analysis was used to determine the conductivity of each complex. Both the 2-PhIm-MSA and 2-MeIm-MSA ionic liquids were found to be less conductive than the Im-MSA complex at base-rich compositions, but more conductive at acid-rich compositions. ^1H -NMR data shows a downfield shift of the proton on nitrogen in 2-PhIm compared to Im, suggesting that other factors may diminish the electronic effects of the electron withdrawing group at base-rich compositions. Further studies examining these effects may well result in increased conductivity for Im-based complexes. Understanding the conductive properties of Im-derivatives due to electronic effects will help facilitate the development of a new electrolyte appropriate for automotive fuel cell use.

INTRODUCTION

As the effects of global climate change are becoming more clear, a changing energy landscape has resulted in an increased demand for alternative energy. An emerging clean-energy technology is the fuel cell, which possesses the potential to replace internal combustion engines in automobile systems. However, fuel cell technology must still be adapted

for high performance in automobiles [1]–[3]. Polymer electrolyte membrane fuel cells (PEMFCs) are particularly strong candidates due to their high energy-conversion efficiency, low operating temperatures, and zero emission potential [4]. However, membrane technology must be modified for fuel cells to run efficiently within vehicles before they are competitive for automotive commercialization.

The distinguishing feature of PEMFCs is the polymer electrolyte, which separates the cathode, anode, and reactants while maintaining high proton conductivity (Figure 1). The most common commercially available fuel cells on the market today employ Nafion®, produced by DuPont®, a perfluorinated sulfonic acid polymer with good thermal and chemical stability as well as high proton conductivity. Since water molecules act as the vehicle for proton transport in the membrane, Nafion® requires constant humidification and an operating temperature below the vaporization point of water (100 °C). Due to inefficiencies in the catalyst performance, a significant amount of heat is generated by the fuel cell. Any excess heat beyond 100 °C must be removed by a cooling system. Current automotive cooling systems are designed to operate around 120 °C, creating an environment that is incompatible with current fuel cells. Recent research has focused on the development of a polymer which conducts protons at a high temperature (>100° C) and low humidity [5]–[8]. The benchmark goal for a practical polymer is set at 0.1 S/cm at 120 °C by the U.S. Department of Energy (DOE).

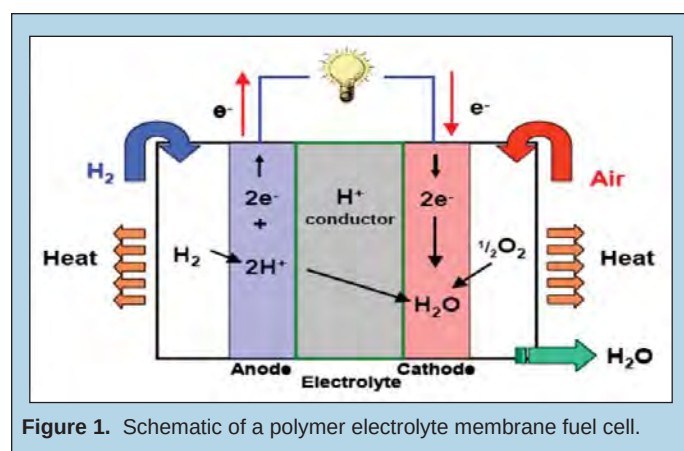


Figure 1. Schematic of a polymer electrolyte membrane fuel cell.

One molecule which has attracted considerable attention as an alternative to water for proton transport is imidazole (Im). Im and its derivatives have been shown to be good Brønsted acids and bases, transporting protons by means of vehicular solvent motion and by the Grotthuss mechanism [9], wherein the protons are transferred by hopping from site to site in a long chain of Im-containing complexes (Figure 2). Unlike Nafion®, Im-based membranes are conductive under anhydrous conditions, demonstrating a potential for the adaptation of fuel cell technology for automotive uses. However, measured conductivities are lower than desired, and the development of a replacement polymer continues. Recent research has investigated several Im-based compounds with various functional groups which could be used at 120 °C and low humidity, but a replacement for Nafion® has not yet been produced [10]–[11].

Considering the laborious process of polymer synthesis, ionic liquids can serve as preliminary compounds upon which polymers may be modeled. Proton-conducting ionic liquids are salts composed of an acid/base pair; they have high proton conductivity but lack the ordered structure provided by a polymer backbone. The acid provides a source of protons while the base, typically a heterocyclic compound, provides a means of proton transfer through solvation. Not only must the acid/base pair be carefully selected but

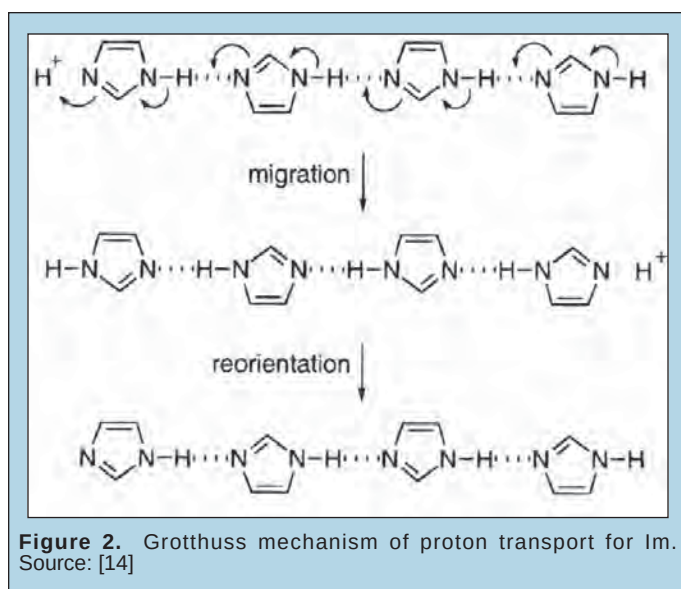


Figure 2. Grotthuss mechanism of proton transport for Im. Source: [14]

proper molar ratios must also be maintained to maximize proton conductivity.

This study examines the effect of electron-withdrawing and electron-donating groups on the conductivity of Im-based ionic liquids. Im, 2-methylimidazole (2-MeIm), and 2-phenylimidazole (2-PhIm) are complexed with methanesulfonic acid (MSA) at defined molar ratios (Figure 3). Altering the electron density of the lone pair on nitrogen may increase the proton accepting and donating potential of Im. Impedance analysis is used to determine the conductivity of each ionic liquid at operating temperatures of 30–130 °C. The thermal properties are determined using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). Proton nuclear magnetic resonance (¹H-NMR) is used to characterize the chemical shift of selected protons.

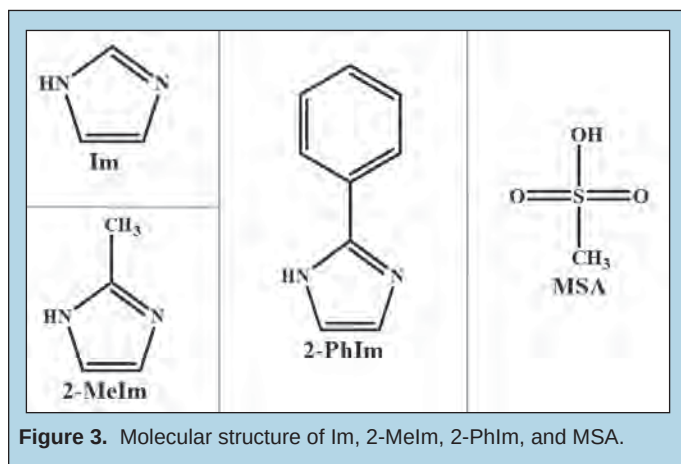


Figure 3. Molecular structure of Im, 2-MeIm, 2-PhIm, and MSA.

The electron donating (methyl) and electron-withdrawing (phenyl) groups are postulated to have different effects on proton conductivity of the complexes they form with MSA. The phenyl group is expected to reduce the electron density of the lone pair on nitrogen. The resulting weaker covalent bonds formed between Im and protons may increase the ease in which Im facilitates proton transport. However, steric hindrance due to bulky substituents could hinder the transfer of protons, thus reducing the overall conductivity. The successful development of an ionic liquid with acceptable proton

conductivity and thermal stability may help fuel cell technology realize its full potential in transforming the automotive industry.

MATERIALS AND METHODS

Im (Fluka, 99.9%), 2-MeIm (Aldrich, 99%), 2-PhIm (Aldrich, 98%), and MSA (Aldrich, 99.5%) were used as received. Mixtures containing predetermined molar ratios of the Im-derivatives and MSA were heated above their respective melting temperatures to ensure homogenization for the ionic liquid complexes. All of the samples were handled and stored in a glovebox with a helium atmosphere.

Thermal Properties

Differential scanning calorimetry (DSC) was performed using a Perkin Elmer Differential Scanning Calorimeter 7 under a helium atmosphere. The samples were sealed in aluminum pans under a helium atmosphere in the glovebox before analysis. Thermograms were recorded during subsequent cooling and heating cycles. The samples were scanned at a rate of $10\text{ }^{\circ}\text{C min}^{-1}$ within the temperature range of $100\text{--}150\text{ }^{\circ}\text{C}$ for base-rich compositions, $50\text{--}250\text{ }^{\circ}\text{C}$ for equimolar compositions, and $150\text{--}100\text{ }^{\circ}\text{C}$ for acid-rich compositions. The melting temperatures (T_m , onset of endothermic peak), crystallization temperatures (T_c , onset of exothermic peak), glass-transition temperatures (T_g), and heat of fusions (ΔH) were determined by the average of two cooling and heating cycles. High temperature stability measurements were conducted using a Perkin Elmer Thermogravimetric Analyzer 7 within the temperature range of $30\text{--}500\text{ }^{\circ}\text{C}$ at a heating rate of $5\text{ }^{\circ}\text{C min}^{-1}$ under a nitrogen atmosphere in open platinum pans.

Ionic Conductivity

The ionic conductivity was determined using an impedance analysis method within the temperature range $130\text{--}30\text{ }^{\circ}\text{C}$ in an oven. The samples were allowed to thermally equilibrate for at least 30 minutes prior to the impedance measurement. The measurements were taken on a cell where the ionic liquid was confined between two stainless steel electrodes separated by a polypropylene spacer. The cell was sealed inside the glovebox. The measurements were performed with a Gamry Instruments Reference 600 Potentiostat/Galvanostat/Zero Resistance Ammeter (ZRA) over a frequency range of $5\text{ }000\text{--}65\text{ }000\text{ Hz}$. The conductivity was calculated from the measured resistance (x-intercept of Nyquist plot) using Ohm's Law.

$^1\text{H-NMR}$ Spectra

The $^1\text{H-NMR}$ spectra were obtained by a Bruker AVQ-400 spectrometer at 400 MHz. Each sample was dissolved in dimethyl- d_6 sulfoxide (DMSO- d_6 , 99.9%-d). The measurements were conducted at room temperature.

RESULTS

The melting temperatures (T_m), crystallization temperatures (T_c), and glass-transition temperatures (T_g) for the Im-MSA ionic liquids obtained by DSC are listed in Table 1. T_m was highest for the equimolar composition at $179.08\text{ }^{\circ}\text{C}$, and a T_g was only present in acid-rich compositions. The heats of fusion of the ionic liquids Im-MSA 5:5, 8:2, 4:6, 2-MeIm-MSA 8:2, 4:6, and 2-PhIm-MSA 8:2, 4:6 are listed in Table 2. The equimolar salt had the highest heat of fusion at 64.23 J g^{-1} ; base-rich compositions had higher heats of fusion than acid-rich compositions. Thermal stabilities at high

temperatures are shown in Figure 4 for Im-MSA ionic liquids. Im-rich compositions showed two step weight losses, the first around $150\text{ }^{\circ}\text{C}$, the second around $300\text{ }^{\circ}\text{C}$.

Mol Fraction Im	$T_m\text{ [}^{\circ}\text{C]}$	$T_c\text{ [}^{\circ}\text{C]}$	$T_g\text{ [}^{\circ}\text{C]}$
1	91.97	46.92	–
0.9	47.76	21.27	–
0.8	61.06	24.86	–
0.7	47.04	17.64	–
0.6	47.38	14.97	–
0.5	179.08	177.62	–
0.4	-6.74	–	–
0.3	–	–	-76.22
0.2	–	–	-88.6
0.1	–	–	-93.88

Table 1. Thermal properties of Im-MSA ionic liquid compositions.

Sample	$\Delta H\text{ [J g}^{-1}\text{]}$
Im-MSA 5:5	64.23
Im-MSA 8:2	19.48
2-MeIm-MSA 8:2	47.67
2-PhIm-MSA 8:2	6.35
Im-MSA 4:6	8.48
2-MeIm-MSA 4:6	1.24
2-PhIm-MSA 4:6	–

Table 2. Selected heats of fusion of Im-MSA, 2-MeIm-MSA and 2-PhIm-MSA ionic liquid compositions.

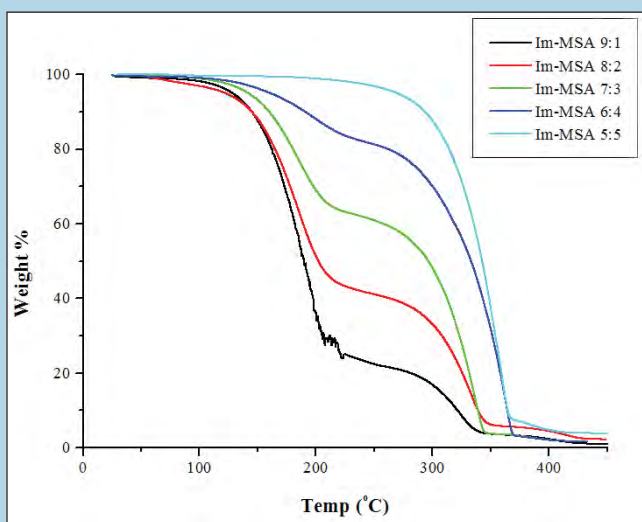


Figure 4. High temperature stabilities for Im-MSA ionic liquids.

The $^1\text{H-NMR}$ spectra for Im-MSA 8:2, 6:4, 4:6 and 2:8 ionic liquids are shown in Figure 5. Four distinct peaks are present, representing the three unique proton environments on Im and the one unique proton environment on MSA. Figure 6 compares the chemical shift of the acidic proton on MSA for Im-MSA, 2-MeIm-MSA, and 2-PhIm-MSA at a 4:6 molar ratio. The proton in the 2-PhIm-MSA complex is farthest upfield, while the proton in the

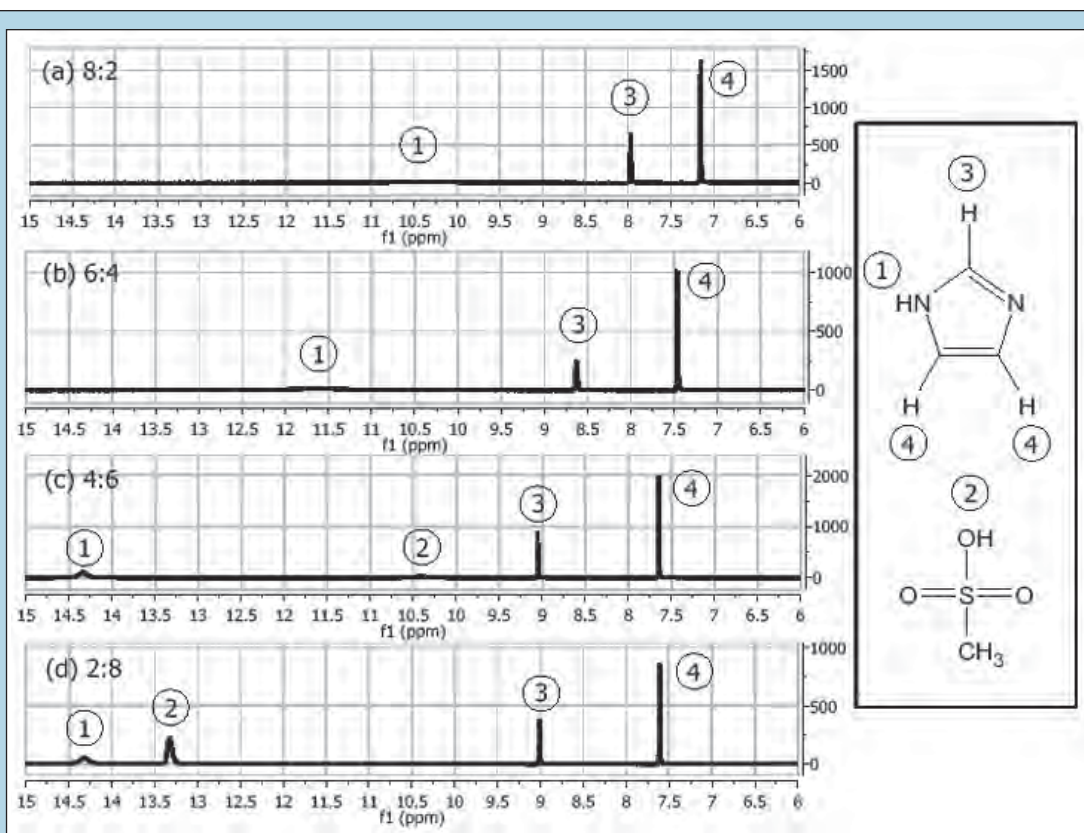


Figure 5. ^1H -NMR spectra for (a) Im-MSA 8:2, (b) Im-MSA 6:4, (c) Im-MSA 4:6 and (d) Im-MSA 2:8 ionic liquids.

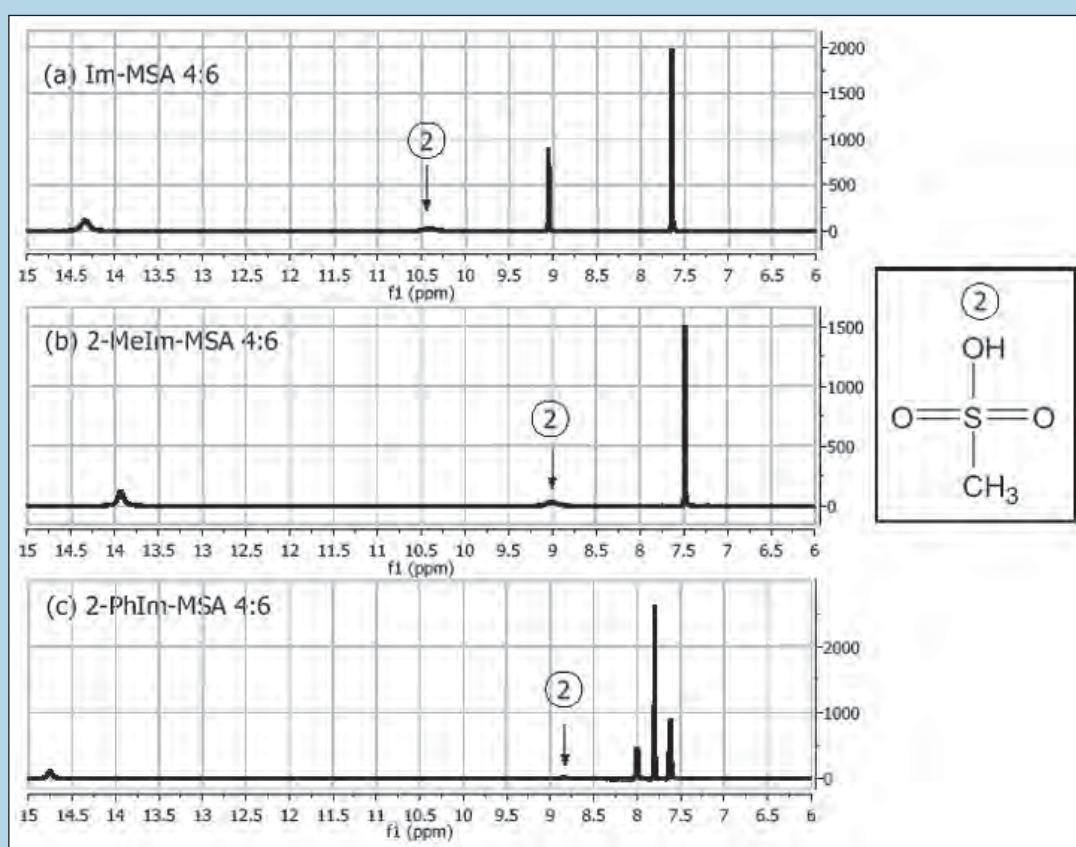
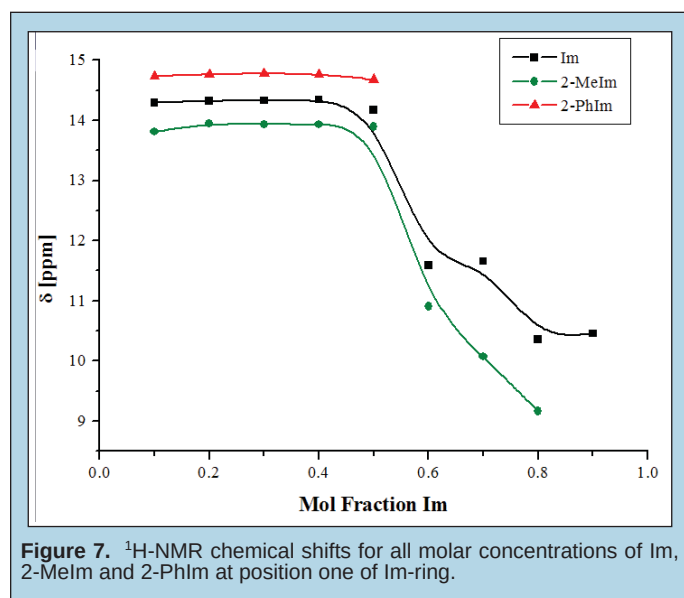
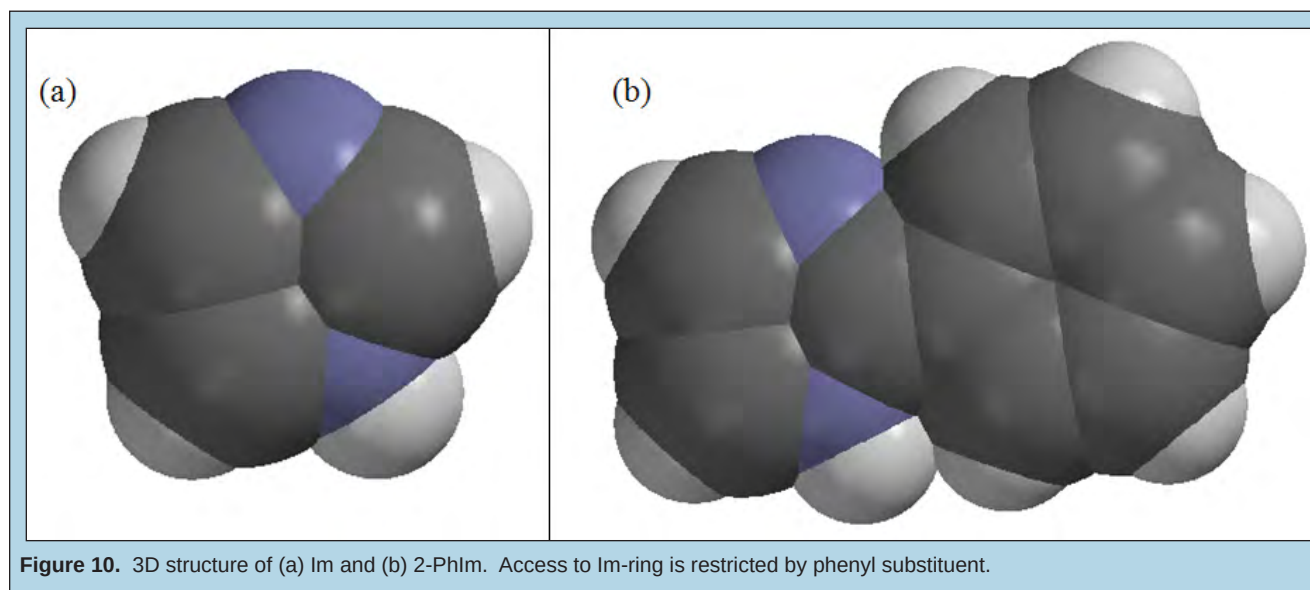
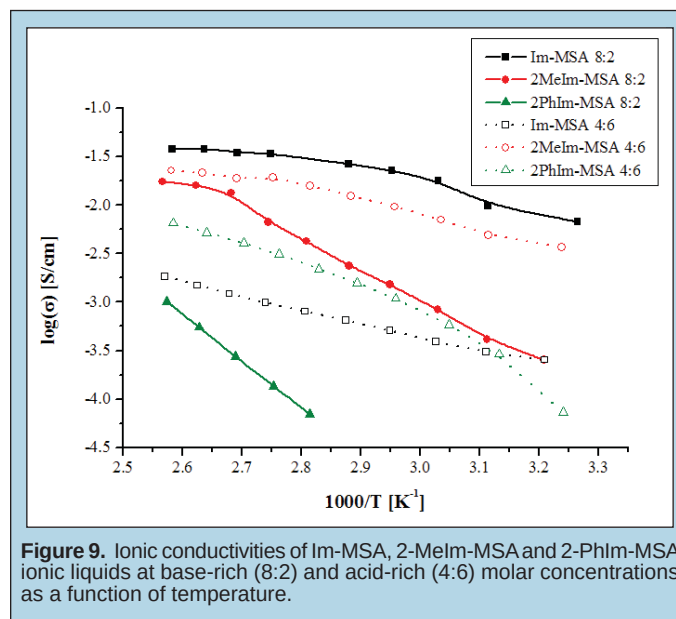
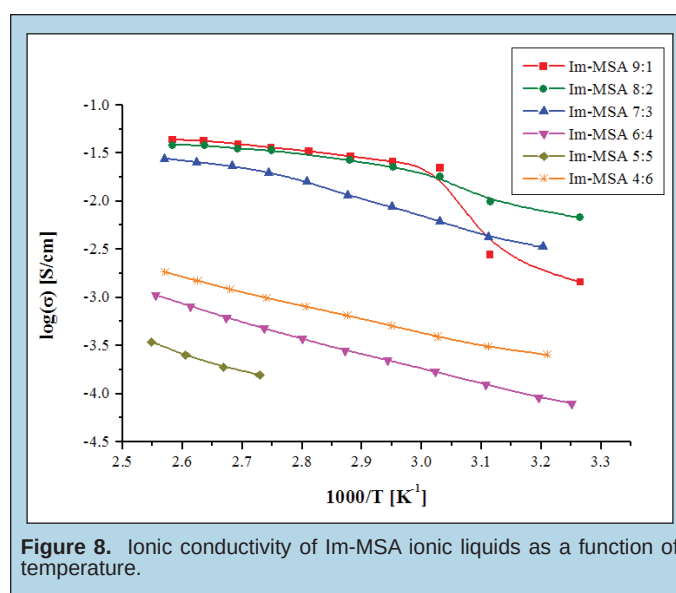


Figure 6. ^1H -NMR spectra for (a) Im-MSA 4:6, (b) 2-MeIm-MSA 4:6 and (c) 2-PhIm-MSA 4:6 ionic liquids.

Im-MSA complex is farthest downfield. Figure 7 compares the chemical shift of the proton at position one of the Im-ring at all molar concentrations of three ionic liquid complexes. In Figure 7, the proton in the 2-PhIm-MSA complex is farthest downfield, while the proton in the 2-MeIm-MSA complex is farthest upfield.



The dependence of ionic conductivity on temperature for all Im-MSA ionic liquid compositions is shown in Figure 8. The maximum conductivity reached was 4.35×10^{-2} S/cm, close to the benchmark goal desired by DOE. Conductivity decreased as temperature decreased, and base-rich compositions were the most conductive. The comparative conductivities of the 8:2 and 4:6 molar ratios of Im-MSA, 2-MeIm-MSA, and 2-PhIm-MSA as a function of temperature are shown in Figure 9. Unlike the Im-MSA complexes, acid-rich compositions of both the 2-MeIm-MSA and 2-PmIm-MSA complexes were more conductive than base-rich compositions. Figure 10 shows the three-dimensional structures of Im and 2-PhIm. Access to Im-ring is restricted by phenyl substituent.



Thermal Behavior

The results from DSC testing showed that the melting point generally varied with molar concentration, and several patterns persist. The pure base maintained a higher melting point than when complexed with acid in unequal molar amounts. However, the equimolar salt had a significantly higher melting point than the other compositions. This result is due to the formation of a pure imidazolium salt with a very ordered crystalline structure, evidenced by the high heat of fusion (Table 2). Base-rich compositions were generally solids at room temperature, having higher melting points than acid-rich compositions, which were generally liquids at room temperature.

Results from the high-temperature stability testing using TGA show the expected weight losses. The equimolar composition showed a one-step weight loss above 300 °C, indicating high thermal stability. Im-rich compositions showed two step weight losses. The step at 150 °C represents the decomposition of excess Im, resulting in an equimolar salt which decomposes in the second step above 300 °C, similar to the 5:5 compositions. A greater molar ratio of Im present in the original salt results in a greater weight loss at the 150 °C step. The results demonstrate that temperature must be kept under 150 °C to maintain a base-rich ionic liquid, otherwise decomposition to an equimolar salt will occur. This data is accurate for ionic liquids only, in which the molecules are highly mobile; the incorporation of these molar ratios into a polymer membrane will change the thermal stabilities of the mixtures by tethering both the Im-ring and acid group to the polymer backbone.

¹H-NMR Chemical Shift

The proton transfer of the Grotthuss mechanism occurs at the number one position on the Im-ring. The chemical shift of this proton is important to understanding the electron density on the nitrogen atom. Figure 5 shows the ¹H signal moves further downfield as the molar concentration of acid increases, indicating that the proton is more localized on the Im-ring in an MSA-rich environment, evidence that the excess acid effectively protonates all the Im. Additionally, the chemical shift of the acidic proton on MSA appears only at MSA-rich compositions where excess MSA is present, shifting downfield and becoming more distinct. This further indicates that all the Im is protonated and the excess MSA does not dissociate.

Comparing the effects of the substituents in Figure 7, the data shows that the proton at position one of the Im-ring of 2-PhIm-MSA is shifted downfield compared to the proton on Im-MSA, while that of 2-MeIm-MSA is shifted upfield. The results confirm that the electron-withdrawing phenyl group attracts electron density away from the Im-ring, while the electron-donating methyl group contributes electron density. Therefore, the Im-ring of 2-PhIm is the most acidic, while the Im-ring of 2-MeIm is the least. The acidity is expected to directly affect the proton conductivity of the ionic liquids; the more acidic 2-PhIm forms weaker covalent bonds with protons, lowering the energy required to transfer that proton to the neighboring molecule.

Ionic Conductivity

A distinction must be made between ionic conductivity and proton conductivity. The methods used in this study measure ionic conductivity, a function of the mobility and concentration of all the charge carriers. The measurements include not only protons but all anions and cations. Therefore, the measured ionic conductivities include the MSA anion. Due to the nature of fuel cell operation, proton conductivity is of critical importance, so comparisons across different molar concentrations and across different bases must be made with consideration to the conductivity of the MSA anion. At acid-rich compositions, the MSA anion will contribute to ionic conductivity more so than at base-rich compositions. Comparisons across different bases must be made at identical molar ratios, to account for the concentration of MSA anions; however, the ionic conductivity cannot be negated. The impedance analysis method requires that an equal volume of ionic liquid be used for each measurement, which results in different molar amounts of acid and base being measured due to the differences in molecular size between Im (68.08 g mol⁻¹), 2-MeIm (82.11 g mol⁻¹), and 2-PhIm (144.2 g mol⁻¹). Therefore, the concentration of charge carriers varies between ionic liquids. With these considerations in mind, the following conclusions can still be drawn about the effect of the methyl and phenyl substituents on the proton conductivity of Im.

As seen in Figure 8, the conductivity of the Im-MSA ionic liquid increases with greater molar concentrations of Im. This result agrees with previous research, concluding that increased mole fractions of Im increase conductivity due to more rapid intermolecular proton transfer between the imidazole molecules [12]. They suggest that the method of proton transport is likely a combination of vehicle and Grotthuss-type mechanisms. The small temperature dependence of the Im-MSA 9:1, 8:2, and 7:3 ionic liquids is consistent with the operation of the Grotthuss mechanism over vehicular motion. Strong temperature dependence is more characteristic of the latter, as seen in the Im-MSA 6:4, 5:5, and 4:6 ionic liquids. Rotation of the Im molecule is less energetic than the movement of a proton carrier, and decreases in temperature have less of a negative effect on the conductivity of ionic liquids dominated by Grotthuss-type transport. Therefore, a shallow slope indicates the operation of the Grotthuss mechanism.

The comparative conductivities in Figure 9 show that the methyl and phenyl substituents affect the conductivity in different ways at base-rich and acid-rich compositions. At the base-rich 8:2 molar concentration, both groups retarded ionic conductivity of the Im-based ionic liquids. The ¹H-NMR shift of N-H in the Im-ring indicated decreased electron density on 2-PhIm-MSA in Figure 7, which is expected to facilitate proton-transfer between 2-PhIm molecules more easily; however, in such a base-rich environment, there is limited accessibility of the Im-ring to protons, a limiting factor in conduction. It must be noted that the phenyl group is significantly more bulky than either a proton or a methyl group; steric hindrance may have affected the accessibility of the nitrogen in the Im ring (Figure 10). As the model shows, access to the nitrogen is severely limited. Table 2 shows that the heat of fusion for 2-PhIm-MSA is lower than the heats of fusion for both Im-MSA and 2-MeIm-MSA, meaning that 2-PhIm doesn't pack as tightly. Therefore, while 2-PhIm may form weaker bonds with protons,

transfer is slowed by the less ordered structure of the ionic liquid, which does not support the Grotthuss mechanism well. Additionally, the phenyl group is less polarizable than the Im-ring, although it is of similar size. Therefore, the dielectric constant of the ionic liquid will be reduced, resulting in greater activation energy to dissociate the proton from MSA. This effect can be seen by a relatively steeper slope of 2-PhIm, which indicates a higher activation energy for conduction.

Interestingly, the conductivities of the acid-rich molar concentrations show a different trend. Both 2-MeIm and 2-PhIm showed increased conductivity over Im. The acid-rich environment produces an excess of protons, eliminating accessibility to protons as a limiting factor. Their great abundance compensates for the steric hindrance produced by bulky substituents, allowing for the electronic effects to predominate. As shown in Figure 7, the ^1H -NMR shift of 2-PhIm occurs farther downfield than Im at acid-rich compositions, confirming that the Im-ring is more acidic; the lowered electron density of 2-PhIm shows the expected result of increased ionic conductivity. The concentration of ions must also be considered. The large size of 2-PhIm reduces the concentration of ion carriers, a factor that reduces the ionic conductivity. Despite this, the 2-PhIm still showed increased conductivity over Im, further supporting the predominance of an electronic effect.

The increased conductivity of 2-MeIm-MSA over Im-MSA is a result that was not expected. A possible explanation is an increase in the number of MSA anions present in the ionic liquid, despite decreased proton conductivity. Figure 7 shows that the ^1H -NMR shift of 2-MeIm is shifted upfield compared to Im, meaning additional electron density increases the strength of the N-H bond, one that is more difficult to break. In the acid-rich environment, the excess of protons ensures that all 2-MeIm molecules are in an imidazolium form. Figure 6 shows that the chemical shift of the acidic proton on MSA is further upfield for 2-MeIm-MSA than for Im-MSA. This result signifies that the proton is more localized on the Im-ring of 2-MeIm, indicating a greater degree of dissociation. Consequently, the concentration of ion carriers is greater in the 2-MeIm-MSA ionic liquid than in the Im-MSA ionic liquid. The increase in ionic conductivity may not be due to increased proton mobility but instead increased ion carrier concentration. However, the 2-MeIm-MSA ionic liquid may facilitate proton transfer more easily because of a highly ordered structure, signified by its high heat of fusion shown in Table 2. Thus, Grotthuss-type proton transport is supported by a tightly packed ionic liquid, but hindered by the increase in electron density on N. Ionic conductivity, however, is increased over Im-MSA because of the higher concentration of ion carriers in the liquid.

CONCLUSION

The most significant discovery of this study is the differing effects of electron-withdrawing and electron-donating groups at base-rich and acid-rich compositions. It is important to note that several factors influence ionic conductivity, including electron density on the Im-ring, the degree of order in the ionic liquid, and the concentration of ion carriers. The ^1H -NMR chemical shifts demonstrate that 2-PhIm is more acidic than Im, which should enhance proton conductivity. However, steric factors become important at base-rich compositions where accessibility to protons

is limited and a lowered dielectric constant increases the activation energy of dissociating the acid. At acid-rich compositions, with sufficient proton availability, the effect of the electron-withdrawing phenyl group predominated, thus increasing conductivity. The electron density on the Im-ring also affects the degree of dissociation of the imidazolium salt and the acid, changing the ion carrier concentration, thus changing the ionic conductivity.

The extension of the results of this study to polymer electrolyte membranes must be made cautiously. Tethering the base and acid groups to a polymer backbone would decrease the ionic conductivity due to the immobilization of ion carriers. The method of proton transport in a polymer structure is limited to a Grotthuss-type mechanism, which will be strictly influenced by the fluidity of protons in an Im-rich environment.

Future studies may help further elucidate electronic properties of such substituents by choosing less sterically-hindered bases, such as 2-chloroimidazole, which the synthesis for is described by [13]. Such a base would reduce the amount of steric hindrance produced by the substituent, as well as maintaining a high dielectric constant which would lower the activation energy of dissociating the acid. Studies using various bases, such as triflic acid, also may help find patterns between electronegativity and conductivity. Greater understanding of the electronic properties of Im-based ionic liquids will aid in the strategic development of a novel polymer with acceptable proton conductivity for use in automotive fuel cells. Such an advance is critical as modern society searches for a clean-burning replacement for fossil fuels.

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PREDICTION METRICS FOR CHEMICAL DETECTION IN LONG-WAVE INFRARED HYPERSPECTRAL IMAGERY

MARIE CHILTON, STEPHEN J. WALSH AND DON S. DALY

ABSTRACT

Natural and man-made chemical processes generate gaseous plumes that may be detected by hyperspectral imaging, which produces a matrix of spectra affected by the chemical constituents of the plume, the atmosphere, the bounding background surface and instrument noise. A physics-based model of observed radiance shows that high chemical absorbance and low background emissivity result in a larger chemical signature. Using simulated hyperspectral imagery, this study investigated two metrics which exploited this relationship. The objective was to explore how well the chosen metrics predicted when a chemical would be more easily detected when comparing one background type to another. The two predictor metrics correctly rank ordered the backgrounds for about 94% of the chemicals tested as compared to the background rank orders from Whitened Matched Filtering (a detection algorithm) of the simulated spectra. These results suggest that the metrics provide a reasonable summary of how the background emissivity and chemical absorbance interact to produce the at-sensor chemical signal. This study suggests that similarly effective predictors that account for more general physical conditions may be derived.

INTRODUCTION

Agricultural, manufacturing and natural chemical processes can generate characteristic gaseous plumes. Nearly every molecular gas has a unique long-wave infrared (LWIR) absorption spectrum. Thus chemical constituents of gaseous plumes can be detected and identified in LWIR hyperspectral images [1]. Chemical detectability depends upon many nuisance factors such as the background type. It may be possible to predict the relative detectability of a chemical as a function of such nuisance factors.

Hyperspectral sensors collect a three-dimensional array of radiance observations. The observed ground area accounts for two dimensions of this image. The third dimension is defined by a wavenumber range of the electromagnetic spectrum. A radiance measurement is the sum of the cumulative effects of the plume gas type, plume gas concentration, atmosphere, background surface, temperature difference between the plume and background, and instrument noise [1], [2].

Plume detection and characterization is a complex problem. Real-world data that lends itself to understanding the physical

phenomenology is almost non-existent. As such, this study uses computer simulations to explore the relationship between the effects of background surface and gas type on the detectability of 499 gases over six distinct backgrounds. The simulated data is produced by a physics-based model. Chemical detections are decided by a Whitened Matched Filter (a detection algorithm) [1]. The objective of this research is to evaluate predictors of relative chemical detectability that are functions of laboratory chemical absorbance and background spectra.

Introduction to the Physics of Radiative Transfer

Sensor-observed radiance can be summarized by a physics-based model that incorporates the effects of the plume gas, background surface, temperature difference between the plume and the ground, and the atmosphere recorded radiance [2]. According to Kirchoff's law, all incident radiation is reflected, absorbed or transmitted by the body it impacts, or $1 = \alpha + \tau + \rho$, where α is the fraction of radiation the body absorbs, τ is the fraction of radiation the body transmits, and ρ is the fraction of radiation the body reflects [3].

Further, Kirchoff's law states that at thermodynamic equilibrium, an object's absorbance is equal to its emissivity (ϵ) defined as the proportion of radiation an object emits to the radiation it would emit as a blackbody at the same temperature. Since a blackbody is an object which absorbs and emits all incident radiation and since no natural object is a perfect blackbody, $0 < \epsilon < 1$ [2].

For optically thin plumes, the transmissivity of the plume (τ_p) can be reasonably approximated by $1 - A(v) \cdot c$ for small c where $A(v)$ is the chemical absorbance in inverse parts-per-million-meter denoted $(\text{ppm-m})^{-1}$ at wavenumber $\nu(\text{cm}^{-1})$ and c is the concentration path length of the gas measured in ppm-m [2]. The expression for radiance recorded by the instrument with a plume present, L_{obs} , can be expressed as the sum of noise and the signal due to each of three layers: plume, ground and atmosphere. Explicitly:

$$L_{obs}(\nu) = \tau_a(\nu) [B(T_p; \nu) - L_g(\nu)] + A(\nu) \cdot c + \tau_a(\nu) L_g(\nu) + L_u(\nu) + e(\nu), \quad (1)$$

is the physics-based model for L_{obs} as a function of wavenumber, ν , where $\tau_a(\nu)$ is the transmissivity of the atmosphere at ν ; $B(T_p; \nu)$ ($\text{W}/\text{cm}^2/\text{Sr}/\text{cm}^{-1}$) is Planck's Blackbody function for radiance at plume temperature T_p (K) and wavenumber ν ; $L_g(\nu)$ is the radiance due to the background surface; $L_u(\nu)$ is the atmospheric up-welling radiance; and $e(\nu)$ represents measurement and modeling error. A graphical representation of Eq. (1) is presented in Figure 1 [2]. The background radiance $L_g(\nu)$ may be expressed as

$$L_g(\nu) = \epsilon_g(\nu) B(T_g; \nu), \quad (2)$$

where ϵ_g is the emissivity of the ground [2]. Note that this expression ignores reflected down-welling radiance because its impact on L_{obs} is negligible [3].

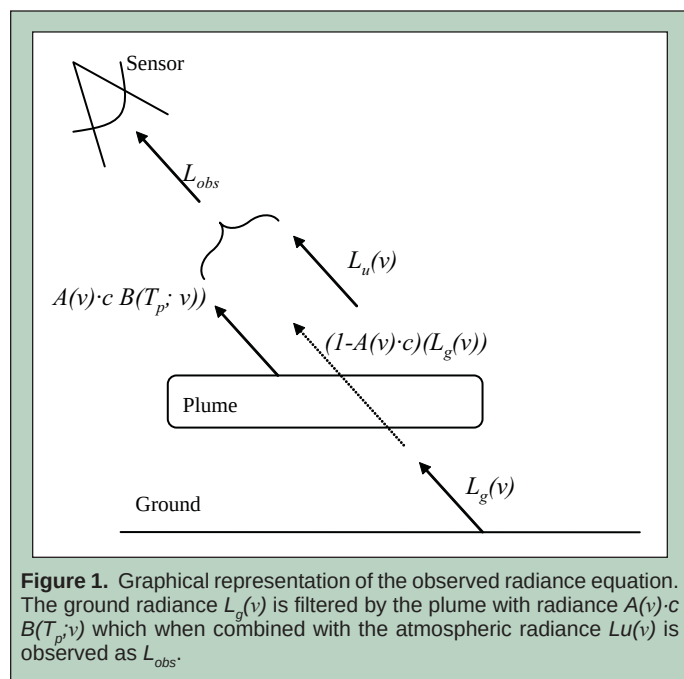


Figure 1. Graphical representation of the observed radiance equation. The ground radiance $L_g(\nu)$ is filtered by the plume with radiance $A(v) \cdot c \cdot B(T_p; \nu)$ which when combined with the atmospheric radiance $L_u(\nu)$ is observed as L_{obs} .

Plume/Ground Temperature Equality

For this paper we studied an admittedly constraining plume/ground temperature case. The intent was to remove the effect of the plume/ground temperature difference on the chemical signal in order to isolate the interaction between background emissivity and chemical absorbance. More general temperature cases may be considered in future work. Setting $T_p = T_g = T$ and substituting Eq. (2) into Eq. (1) yields a simplified expression of the physics-based model that more clearly shows the relationship between background emissivity and chemical absorbance:

$$L_{obs}(\nu) = \tau_a(\nu) [B(T; \nu) [1 - \epsilon_g(\nu)]] + A(\nu) \cdot c + \tau_a(\nu) L_g(\nu) + L_u(\nu) + e(\nu). \quad (3)$$

Note that the signal due to the chemical effluent is the first term on the right hand side of Eq. (3), explicitly:

$$\tau_a(\nu) [B(T; \nu) [1 - \epsilon_g(\nu)]] A(\nu) \cdot c. \quad (4)$$

Expression (4) shows that a relatively larger gas absorbance, $A(\nu)$, and a background emissivity, $\epsilon_g(\nu)$, close to 0 (or, equivalently a background reflectance, $1 - \epsilon_g(\nu)$, close to 1) contribute to a relatively larger chemical signal in $L_{obs}(\nu)$ and in turn to relatively higher gas detection probability. We used this reasoning to produce summary measures using chemical absorbance and background emissivity.

Predictors

Based on the intuition gained from the physics-based model, two predictors were explored for their ability to summarize when a chemical may be better detected over one background type versus another. One predictor (M_1) uses each background's reflectance ($1 - \epsilon_g$) at the wavenumber where the absolute maximum chemical absorbance occurs to rank order backgrounds, i.e.

$$M_1 = 1 - \epsilon_g(\nu^*) \text{ where } \nu^* = \arg \max_{\nu} A(\nu). \quad (5)$$

Eq. (3) suggests that the background with the largest M_1 for a given chemical will yield the largest $L_{obs}(\nu^*)$. The dominance of the maximum gas absorbance on detection for a given background is explored with this metric.

Though the chemical absorbance is approximately zero at most wavenumbers, many chemicals may have multiple relative maxima where $\epsilon_g(\nu)$ is also low and these also contribute to the radiance spectrum recorded by the instrument. As such, a predictor that accounts for the chemical absorbance and background emissivity across the whole spectrum is also explored. This predictor sums the products of the squared chemical absorbance and squared background reflectance at each observed wavenumber in the LWIR. It also normalizes the given chemical absorbance spectrum by dividing by its squared magnitude. This predictor is denoted M_2 and is given by:

$$M_2 = \frac{\sum_{i=1}^n (A_i)^2 (1 - \epsilon_{g_i})^2}{\sum_{i=1}^n (A_i)^2}, \quad (6)$$

where n represents the number of wavenumbers (or number of observed spectral channels). Chemical absorbances and background emissivities that generally contribute to larger $L_{obs}(\nu)$ over all wavenumbers tend to give larger values of M_2 .

As an example of how M_1 and M_2 would rank order backgrounds for a specific chemical, the chemical absorbance spectrum of carbon tetrachloride (CCl_4) using the background emissivity spectra of a Paint representative and an Asphalt-Concrete-Soil representative (ACS) are plotted in Figure 2. The absolute maximum of CCl_4 occurs at wavenumber 794 and at that wavenumber, Paint has a greater reflectance ($1 - \epsilon_g$) than ACS so M_1 would order the backgrounds as Paint and then ACS for CCl_4 . Similarly, M_2 for CCl_4 and Paint is 7.499×10^{-3} while M_2 for CCl_4 and ACS is 1.689×10^{-3} . Thus M_2 would also order these backgrounds as Paint and then ACS for CCl_4 . The background orderings as decided by these predictors will be compared to the actual background orderings as decided by a commonly applied chemical detection algorithm.

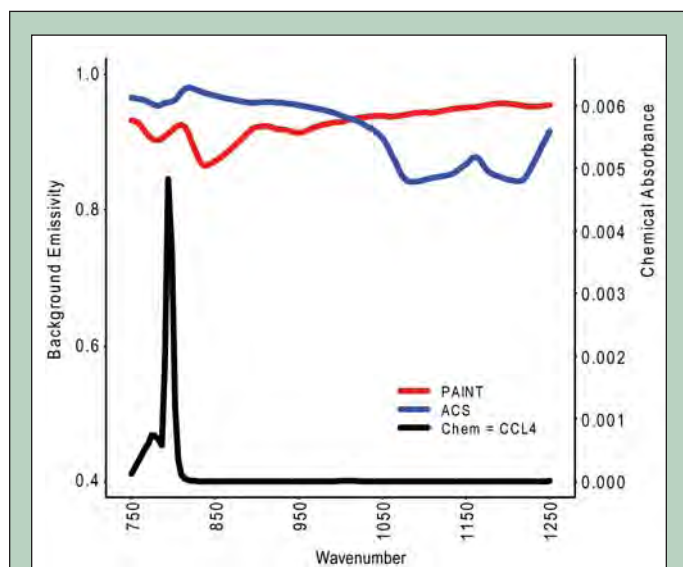


Figure 2. Chemical absorbance spectrum of CCl_4 with PAINT and ACS background emissivity spectra. The difference between PAINT and ACS over the wavenumbers with highest CCl_4 absorbance predicts that CCl_4 would be more easily detected over PAINT than ACS.

Both predictors focus on chemical absorbance and background emissivity, assuming the other variables in the physics-based model, Eq. (3), are held constant. In actual and simulated hyperspectral images, the other variables and noise can also perturb gas detectability. Future work may consider more general plume/ground temperature cases as well as incorporating the atmospheric transmissivity in more generalized predictors.

METHODS

It would be ideal to generate hyperspectral images in the natural environment where all variables could be controlled and manipulated to compare relative detectability of various chemicals over specific backgrounds. However, since this level of control would be extremely difficult and costly (or unattainable) in a real experiment, analysis of computer-simulated data was conducted instead. This allows the relationship between chemical absorbance and background emissivity to be better understood, especially as it relates to gas detectability. We do this by comparing detection results on the simulated hyperspectra to the background orderings as decided by M_1 and M_2 .

This experiment used the InfraRed Systems Analysis in General Environments code (IR-SAGE) developed at Pacific Northwest National Laboratory (PNNL) [4] to simulate LWIR hyperspectra of simplified gaseous plumes over organized background pixels. IR-SAGE uses the physics-based model in Eq. (1) to simulate a radiance vector from the LWIR using a chemical absorbance spectrum, a background emissivity spectrum and atmospheric conditions, while perturbing these quantities with Gaussian noise [4]. Gas absorbance spectra from the PNNL library [6] were used for image simulation. Background emissivity spectra used in the IR-SAGE images were selected from the Nonconventional Exploitation Factors Data System (NEFDS) [7]. Six distinct background emissivities were chosen for image simulation. These emissivities exhibit different behavior across the LWIR spectrum.

One 36-part data cube was simulated for the 499 distinct gases in the library. For all images, the temperature of the plume was set equal to the temperature of the ground so that $T_p = T_g = 300\text{K}$. The spectral range used was 750 to 1250 cm^{-1} in steps of four which yielded a total of 126 spectral channels. Each 36-part cube had dimensions of $150 \times 120 \times 126$ (rows by columns by spectral channels). Each set of 25 rows represented one of the six distinct background types: Asphalt-Concrete-Soil (ACS), Brick, Miscellaneous (MSC), Paint, Snow and Steel and Copper tubing (STCOP). Each set of 20 columns corresponded to a different gas concentration path-length: 16, 8, 4, 2, 1 and 0 ppm-m. Thus each $25 \times 20 \times 126$ part contained 500 replicate pixels for one of the 36 background/gas concentration combinations.

We used a Whitened Matched Filter (WMF) as the gas detection tool [1]. Radiance due to background was first removed from a plume pixel by computing the mean of all ppm-m concentration pixels and then subtracting it from the plume radiance:

$$L_w = L_{on} - \bar{L}_{off} \quad (7)$$

Here, L_w , L_{on} and $\bar{L}_{off}$ are radiance vectors of length 126. Therefore, L_{on} represents a plume pixel and L_w represents the radiance due to the plume and noise after removing the background radiance. These “whitened” spectra were then processed with the WMF. The expression for the scalar WMF can be written as

$$WMF = (A' \hat{\Sigma}^{-1} A)^{-1} A' \hat{\Sigma}^{-1} L_w \quad (8)$$

where A is the chemical absorbance spectrum (vector of length 126) and $\hat{\Sigma}$ is the covariance matrix of the off-plume pixels with dimensions 126×126 . Eq. (8) emphasizes the strength of the chemical signal in L_w while diminishing the effects of noise through the use of $\hat{\Sigma}^{-1}$. In practice, large values of the WMF provide evidence for gas detection [2]. The filter was applied to each pixel. It was necessary to pick a threshold in order to label a pixel as a chemical detection or non-detection. Thus a gas was “detected” in a pixel if WMF was statistically different from zero at the 0.05 significance level [5]. The proportion of gas detections, denoted by $\hat{p}$, out of the 500 replicate pixels was used as an estimate of the gas detection probability for each background type. Backgrounds were ordered for each chemical based on these $\hat{p}$ values. An example of a detection proportion curve for the CCl_4 image is presented in Figure 3. The detection proportions are plotted as a function of gas concentration path-length. There is one $\hat{p}$ curve for each of the six backgrounds. This plot indicates that CCl_4 was best detected over Paint and

worst detected over Snow. The data presented in Figure 3 is used to order the backgrounds for best-to-worst detectability of CCl_4 . This plot gives the ordering as: Paint, STCOP, MSC, Brick, ACS and Snow. Recall the previous examples of predictor metrics. For CCl_4 , M_1 and M_2 both ordered two of the backgrounds as Paint and then ACS. We note that these background orderings correspond to the relative ordering of Paint and ACS for CCl_4 as decided by the WMF detections.

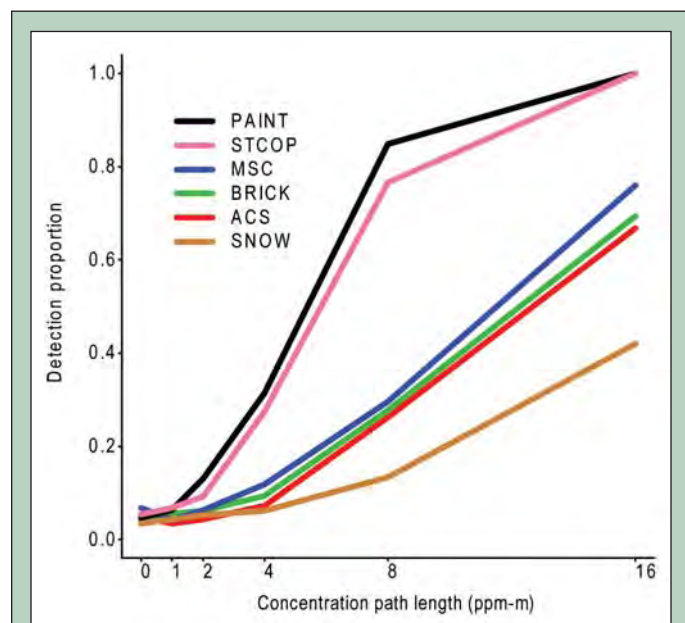


Figure 3. Example detection proportion curves from simulated image of CCl_4 plume. In the simulation, CCl_4 was more easily detected using WMF over PAINT, than STCOP, MSC, BRICK, ACS and finally SNOW, respectively.

Metrics M_1 and M_2 were calculated for all chemical/background combinations using the chemical absorbance spectra from the PNNL gas library and the six aforementioned background emissivity spectra. These metrics gave a ranking of the background types for each chemical. Recall that the physics-based model indicates that, for a given chemical, backgrounds that yield relatively larger scores for M_1 and M_2 will tend to yield relatively larger chemical signals and hence relatively higher detection proportions. Thus for a given chemical, the background orderings as indicated by $\hat{p}$, M_1 and M_2 were interrogated for consistency. We interpret high consistency in these rank orderings as an indication that M_1 and M_2 provide reasonable summaries of how gas absorbance and background emissivity interact to produce the at-sensor observed chemical signal and in turn provide good predictive ability to describe when a chemical will be more easily detected over one background as compared to another.

RESULTS AND DISCUSSION

Initial inspection of the detection results using the Whitened Matched Filter for the 499 images revealed that 276 chemicals had $\hat{p}$ values less than 0.2 across all backgrounds and concentrations. For these chemicals, the detection proportion curves were not separated enough to decide how the backgrounds should be rank ordered. This was attributed to a relatively low and flat chemical absorbance across the LWIR (relative to the chemicals that gave

overall large detections). These gases would require simulations that used larger concentration path lengths than those considered to produce informative detection curves. As such, these gases were removed from the study.

For the remaining 223 chemicals, the consistency in background rank orderings among $\hat{p}$, M_1 and M_2 is summarized in Figure 4. Results are shown in a composite bar chart that displays the proportion of rankings that agreed for all three measures (blue), the proportion of rankings that agreed between $\hat{p}$ and M_1 only (yellow), the proportion of rankings that agreed between $\hat{p}$ and M_2 only (orange) and the proportion of rankings that did not agree among all three measures (red). The chart in Figure 4 indicates that M_1 and M_2 were each able to correctly rank order the backgrounds (as compared to the rankings decided by $\hat{p}$) for over 90% of the chemicals. Comparison of the yellow and orange regions of the bars indicates marginal difference in the abilities of M_1 and M_2 to correctly rank order the backgrounds. These results indicate that both M_1 and M_2 are competitive predictors for when a chemical will be better detected over one background type or another. These results hold only for these data and the assumptions we have applied to the physics-based model.

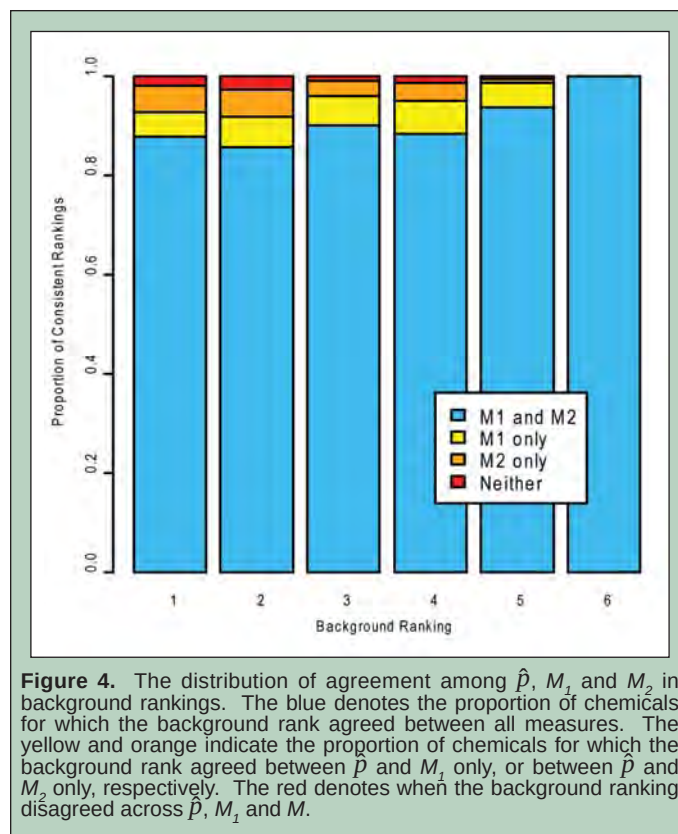


Figure 4. The distribution of agreement among $\hat{p}$, M_1 and M_2 in background rankings. The blue denotes the proportion of chemicals for which the background rank agreed between all measures. The yellow and orange indicate the proportion of chemicals for which the background rank agreed between $\hat{p}$ and M_1 only, or between $\hat{p}$ and M_2 only, respectively. The red denotes when the background ranking disagreed across $\hat{p}$, M_1 and M_2 .

CONCLUSION

Based on the physics-based model, high chemical absorbance and low background emissivity contribute to high gas detectability assuming other variables and noise are held constant. Two predictors were developed to investigate the implications of the physics-based model: one predictor accounted for chemical absorbance and background emissivity at a single wavenumber and the other predictor accounted for these properties across the LWIR spectrum.

Backgrounds were rank ordered based on these predictors for each chemical and compared with the background ordering for gas detection from simulated experimental results.

Simulating and analyzing all 499 data cubes took approximately 72 cpu hours and introduced computational problems because of the size and complexity of each file. Additional sets of data cubes for different conditions would have required too great an amount of cpu time to analyze. These time constraints limited our study to the one plume/ground temperature case: $T_p = T_g$. Plots of chemical absorbance spectra compared to their $\hat{p}$ values suggest that the low magnitude of absorbance spectra was a factor in preventing the other 276 chemicals from being detected in this simulation. This suggests that many of these chemicals would be detectable at higher concentrations. This was not further explored due to time constraints.

Alone, M_1 and M_2 each correctly rank ordered the backgrounds for more than 90% of the 223 chemicals. Even though M_1 focuses only on the chemical absorbance and background emissivity at a single wavenumber, M_1 and M_2 yield similar results. However, M_1 is much simpler computationally and thus it may be considered a better summary metric for these data.

These results are encouraging and suggest that M_1 and M_2 adequately summarize how the background emissivity and chemical absorbance work in conjunction to produce the chemical signal and are good predictors for when a chemical may be better detected over one background type as to another. Future work will attempt to generalize M_1 and M_2 with the aim of incorporating other physics-based parameters and a wider set of conditions on the plume/ground temperatures.

ACKNOWLEDGEMENTS

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TITANIUM DIOXIDE TRIADS FOR IMPROVED CHARGE-SEPARATION USING CONDUCTIVE POLYMERS

TIFFANY M. COCHRAN, TASHA N. GAYLOR, LINDA DE LA GARZA AND TIJANA RAJH

ABSTRACT

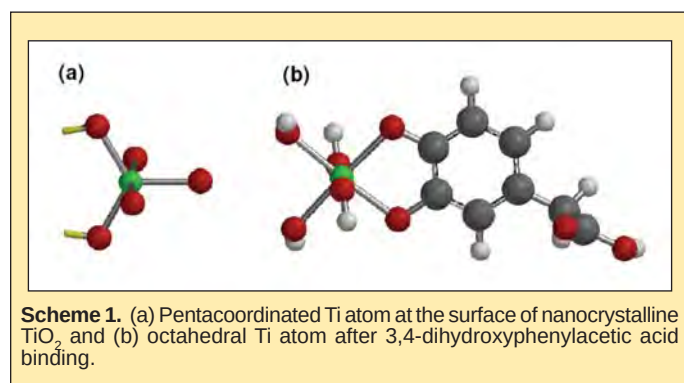
Dye-sensitized solar cells are potentially one of the best solutions to solar energy conversion because of the low cost of required materials and production processes. Titanium dioxide (TiO₂) nanoparticulate films are the basis for one of these types of cells, providing large surface area for dye-sensitizer adsorption. Because TiO₂ nanoparticulate films develop defects caused by oxygen deficiency, deep reactive electron traps are formed. With the addition of an enediol ligand, these electron traps are deliberately removed, enhancing the conduction of electrons within the film. In this project, TiO₂ nanoparticulate films made by a layer-by-layer dip coating method were modified with 3,4-dihydroxyphenylacetic acid (DOPAC). DOPAC binds to the titanium atoms on the surface of the nanoparticles, restoring their octahedral geometry. This restructuring of the surface shifts the spectral properties of the TiO₂ to the visible spectrum and improves the separation of charges which is observed using photoelectrochemistry. Furthermore, DOPAC enables the electronic attachment of other molecules to the surface of TiO₂ films, such as the conductive polymer polyaniline base. This conductive polymer provides an extended separation of charges which increases photocurrent production by forming a triad with the TiO₂ semiconductor through the 3,4-dihydroxyphenylacetic acid linker. The photocurrent increases due to the donor properties of the conductive polymer thereby decreasing charge pair recombination.

INTRODUCTION

The use of dye-sensitized solar cells is one of several means to fulfill the future demand for energy [1], [2]. During illumination electrons from the photoexcited dye are injected into the conduction band of a nanoparticulate semiconductor, such as titanium dioxide (TiO₂). Titanium dioxide is an excellent candidate for a

dye-sensitizer support because of its low cost and optimal redox properties. However, in order to enable high efficiency of light conversion, a large surface area of nanoparticle films is required. An approach to enlarging the surface area of the nanoparticles includes fabricating thicker films using a layer-by-layer deposition of particles in nanoscale regime [3], [4]. These particles, however,

have a truncated surface that undergoes surface reconstruction due to the high curvature of TiO_2 in nanosize regime [5]. As a consequence, the crystal units at the surface of TiO_2 particles result in different spacing of the surface atoms compared to those within the bulk of the nanoparticles. Because of their weaker bonding, the energy level of the surface specie is found in the mid-gap region, thus decreasing its reducing/oxidizing abilities [6]. Therefore, the surface titanium (Ti) atoms act as electron carrier trapping sites that limit the exchange of electrons. Electron traps of TiO_2 arise from oxygen deficiencies and absorbed species on the surface of the film. Selectively, these electron traps can be removed by modifying the surface of Ti atoms with enediol ligands, greatly improving the charge-transfer of electrons by forming a charge-transfer complex [7]. The ligands bind to the surface trapping sites and selectively modify the energetics of the surface Ti atoms by restoring their octahedral coordination as shown in Scheme 1 for a pentacoordinated Ti atom at the surface of nanocrystalline TiO_2 and the octahedral Ti atom after 3,4-dihydroxyphenylacetic acid (DOPAC) binding, forming the charge-transfer complex TiO_2/DC .

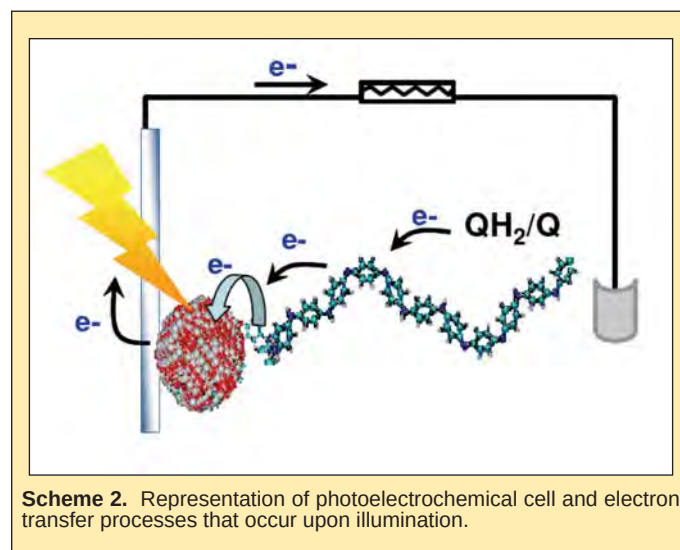


Upon binding, a ligand-to-metal charge transfer (CT) complex forms and the onset of absorption is shifted to the red due to the narrowing of the band-gap of the new hybrid TiO_2 -ligand, allowing more absorption of photons from the visible spectrum. The absorption of these photons yields photo-induced currents [8] which have been measured from bio-inspired assemblies using semiconductor triads and biomolecules such as DNA and proteins that have been linked through the enediol ligand to the semiconductor particles. During illumination, these assemblies act as sequential electron donors showing the feasibility and versatility of the systems [9], [10].

Here, we explore the linkage of conductive polymers to the enediol ligand DOPAC as a method for modifying the surface of TiO_2 nanoparticles. Conductive polyaniline is a promising conductive polymer due to its high conductivity and stability, and it has been previously used in dye-sensitized solar cells. Conductive polymers have been deposited on top of TiO_2 films and shown to produce photocurrents [11], [12], [13]. In this work, the carboxylic acid present in DOPAC is used to attach a conductive polymer, polyaniline base (PANI) to the surface of titanium dioxide nanoparticles forming a conductive-polymer based semiconductor triad. In the conductive-polymer TiO_2 triad, PANI works as a consecutive electron donor providing a channel for hole transport, extending the separation of charges and enhancing the performance

of TiO_2 films. A representation of the photoelectrochemical cell used in this work and electron transfer processes that occur upon illumination is shown in Scheme 2. First, light absorption by the charge-transfer complex TiO_2/DC results on electrons injected in the TiO_2 nanoparticulate film which are then collected at the support electrode. The hole in DOPAC is filled by electron transfer from the PANI and the hydroquinone in solution donates electrons to the oxidized PANI.

Electron paramagnetic resonance (EPR) experiments confirm the extended charge separation on these conductive-polymer based triads. The EPR results will be published elsewhere.



MATERIALS AND METHODS

Fabrication of the Electrodes

Corning 1737 Aluminosilicate Glass Indium Tin Oxide (ITO) electrodes were cleaned in a series of baths which were as follows: 1:1 acetone/methanol solution, cleaning detergent, 20% H_2SO_4 , and finally 0.2 M NaOH in a 1:1 water/methanol solution. After being thoroughly cleaned, the slides were stored in deionized Nanopure water. For experiments, the slides were removed and dried. After drying, the absorbance of each slide was determined using a Shimadzu UV-160 UV Visible Spectrophotometer. A dip-coating method [8] was used to fabricate TiO_2 films from 0.3 M TiO_2 colloidal solution with 5 nm particle size [7] mixed 1:1 with an amphiphilic triblock copolymer of ethylene oxide and propylene oxide aqueous solution (20% Pluronic) [14]. The non-conductive side of the electrode was covered with adhesive tape, to expose only the conductive side to the solution. Electrodes were dip-coated three times each to cover about three-quarters of the area. Each electrode was then dried in an oven at 150 °C for 30 minutes before the next coat. Finally, the electrodes were annealed at 450 °C for one hour under a constant stream of oxygen. After annealing, contacts were added. Each contact was a strand of nickel wire, coiled on one end and coated with silver paint. The coiled-silver-coated end of the wire was placed directly onto the conductive side of the electrode on the end where there was no TiO_2 coating present. The wire was attached by wrapping adhesive tape around it.

Photocurrents

Photoelectrochemical measurements were carried out in a 40 mM phosphate buffer solution at pH 6.8 that contained 5 mM hydroquinone as the redox relay. Nitrogen gas purged the oxygen from the system. A Bioanalytical Systems Analyzer (BAS 100B) was used to measure the photocurrents in the three-electrode cell. The reference electrode was Ag/AgCl (0.2 V vs. NHE, normal hydrogen electrode), the working electrode was the fabricated TiO₂ electrode, and a platinum wire was used as the counter electrode. Photocurrents are reported as the difference in current with and without incident light on the backside of the TiO₂ electrode. Monochromatic light was provided by a Jobin-Yvon grating monochromator in line with an ILC Technology xenon arc lamp. Each electrode was tested individually and exposed to light during five seconds at different wavelengths. The light intensity of the lamp was ~25 mW/cm² at a 400 nm wavelength.

Modification of TiO₂ Electrodes with Eneiol Ligand

To modify the TiO₂ electrodes, films were immersed in a 20 mM eneiol ligand (DOPAC) aqueous solution for two hours within a N₂ glovebox. Electrodes were kept in the dark unless in use.

Modification of TiO₂ Electrodes with PANI-Based Conductive Polymers

The carboxyl groups of DOPAC were activated using 50 mg/mL 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride and 100 mg/mL of N-hydroxy-succinimide in a 0.05 M MES buffer pH 6.8 (MES hydrate minimum 99.5% Titration, SIGMA C₆H₃NO₄S) mixed in a 10 mM DOPAC solution [3]. After being activated, 500 μ L of polyaniline (1 mM PANI 5000) in dimethylformamide (DMF) were added to 250 μ L of the activated DOPAC solution and allowed to react for two to four hours. Then it was put into dialysis tubing to eliminate non-reacting material, and it was dialyzed in solution of 1:1 DMF/H₂O twice for six to ten hours each time. The final solution used for TiO₂ surface modification was 0.1 mM DOPAC. After dialysis, 100 μ L of solution were placed on each electrode for two hours and allowed to react under a N₂ atmosphere in the dark. Afterwards, the electrodes were washed with N₂-purged H₂O.

RESULTS AND DISCUSSION

Nanoparticulate TiO₂ was deposited using the dip-coat method on ITO slides to produce ITO/TiO₂ electrodes. To confirm TiO₂ nanoparticle deposition on ITO, absorbance spectra of the electrodes were recorded before and after deposition using an empty quartz cuvette as background (Figure 1).

After deposition, there was an enhancement of absorption between 250 and 350 nm, corresponding to the band gap absorption of TiO₂ adsorbed on ITO. Depending on the film thickness, additional features that originated from interference of light by thin film nanoparticles were observed in the spectra. The ITO/TiO₂ electrodes were then modified with 3, 4-dihydroxyphenylacetic acid, DOPAC (TiO₂/DC) by soaking the electrode in 20 mM DOPAC aqueous solution for two hours. As shown in Figure 2, there was a shift of the onset of absorption to the red part of the spectrum after surface modification.

An aqueous DOPAC solution does not have absorption at wavelengths higher than 350 nm. The shift in the absorption was

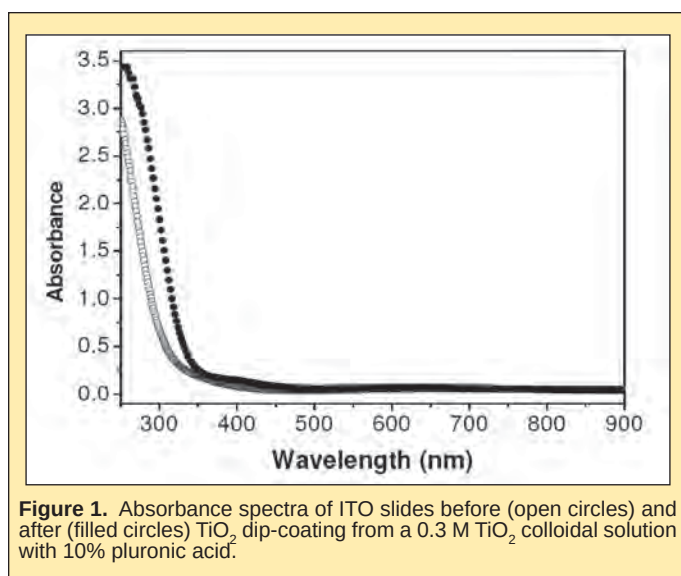


Figure 1. Absorbance spectra of ITO slides before (open circles) and after (filled circles) TiO₂ dip-coating from a 0.3 M TiO₂ colloidal solution with 10% pluronic acid.

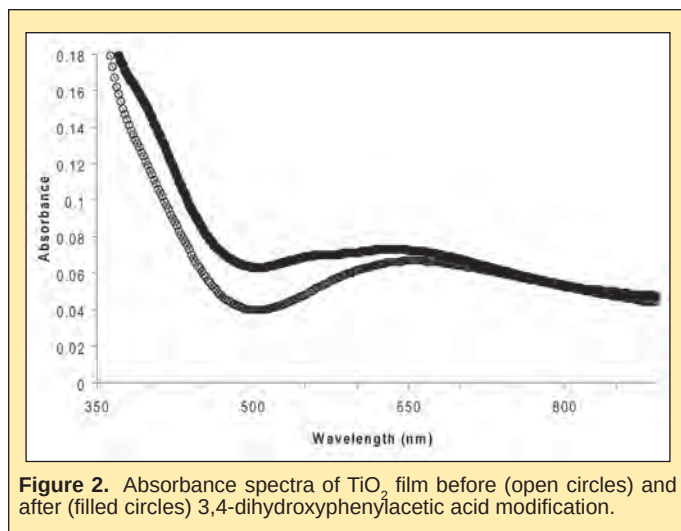


Figure 2. Absorbance spectra of TiO₂ film before (open circles) and after (filled circles) 3,4-dihydroxyphenylacetic acid modification.

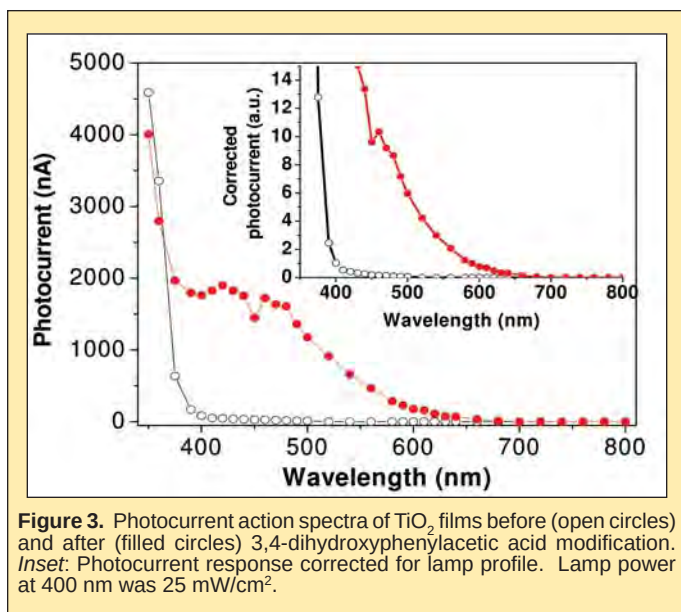
due to the excitation of localized electrons from the DOPAC into the conduction band of the semiconductor particle, prompting the formation of the charge-transfer complex on the surface of the TiO₂/DC films [7], [15].

Photocurrent action spectra of DOPAC-modified electrodes were measured and reflect the dependence of charge-transfer efficiency on the wavelength of absorbed light as shown in Figure 3.

Photocurrents were measured from 350 nm to 800 nm at 10–20 nm intervals for electrodes before and after modification. The photocurrent responses corrected for the lamp profile are shown in Figure 3's inset. Corrected photocurrents (incident-photon-to-current-efficiencies, IPCE) were calculated from photocurrent measurements using the formula below, where $I_{h\nu}$ is the photocurrent calculated from the light minus dark cycles, λ is the incident light wavelength and P is the power of the lamp at that wavelength⁸:

$$\text{IPCE} = 1.24 * I_{h\nu} (\mu\text{A}) / \lambda (\text{nm}) * P (\text{mW})$$

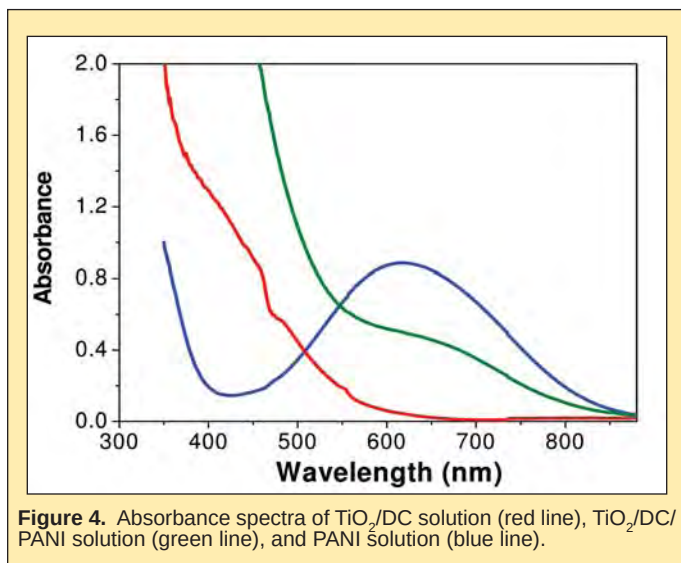
Absorption of light by the TiO₂/DC charge-transfer complex promotes electrons from the DOPAC ligands to the conduction band of the TiO₂ particles, and photocurrent arises upon their subsequent collection by the conductive ITO substrate. The photocurrent



produced by the modified films mirrors the absorption spectra, as can be seen by comparing Figure 2 and the inset of Figure 3. For bare TiO_2 films, photocurrent production was mostly detected at wavelengths shorter than 400 nm, while photocurrent production for TiO_2/DC films starts in the visible range, indicating that the TiO_2/DC charge-transfer complex is producing the current under illumination.

Semiconductor Triads Based on Conductive Polymers

For the following experiments, the ITO/ TiO_2 electrodes were modified by soaking in a solution containing DOPAC and DOPAC-linked-PANI obtained from the coupling reaction as described in the methods. Due to the synthesis followed, the concentration of the solution used for soaking the electrode was only 0.1 mM resulting in a lower photocurrent compared to that of the 20 mM DOPAC concentration. Absorbance spectra of solutions of TiO_2/DC , $\text{TiO}_2/\text{DC}/\text{PANI}$ and PANI are shown in Figure 4.



PANI in solution has a broad absorbance band in the visible range (from 400 to 900 nm) with a maximum around 620 nm. In the triad $\text{TiO}_2/\text{DC}/\text{PANI}$ the band is still present but now along with the charge-transfer complex of TiO_2/DC , thus forming a composite spectrum. Absorbance spectra of TiO_2 films were recorded before and after surface modification (Figure 5).

Absorbance differences shown in Figure 5d for comparison purposes show a slight increase in absorbance around 400 nm for the TiO_2/DC electrode and a broad increase in absorbance for the $\text{TiO}_2/\text{DC}/\text{PANI}$ electrode, similar to the TiO_2/DC and $\text{TiO}_2/\text{DC}/\text{PANI}$ spectra in solution. During illumination with visible light, TiO_2/DC and $\text{TiO}_2/\text{DC}/\text{PANI}$ gave rise to wavelength-dependent photocurrents which resembled the absorption of the TiO_2/DC modified particles. Photocurrent action spectra for all unmodified electrodes were very similar, so only one is shown in Figure 6.

After surface modification, photocurrent action spectra of the modified films were measured and reflected the dependence of charge transfer efficiency on the wavelength of absorbed light and how well the particles in the film are connected after annealing. When light is absorbed by the TiO_2/DC charge-transfer complex, it enables electrons to move from the DOPAC ligands to the conduction band of the titanium particles, followed by collection by the conductive ITO substrate. The $\text{TiO}_2/\text{DC}/\text{PANI}$ electrode gave rise to larger photocurrent production in the same wavelengths as the TiO_2/DC film. The photocurrents corrected by the lamp profile are shown in Figure 7.

The corrected action spectra of the TiO_2/DC and $\text{TiO}_2/\text{DC}/\text{PANI}$ electrodes have the same wavelength dependence of photocurrents indicating that the charge-transfer of TiO_2/DC is responsible for photocurrent production without PANI acting as a sensitizer. Nevertheless, the efficiency values of $\text{TiO}_2/\text{DC}/\text{PANI}$ electrodes are about three times higher than that of TiO_2/DC , showing the improved photoconversion efficiency of the semiconductor triad. The $\text{TiO}_2/\text{DC}/\text{PANI}$ electrode has even a higher efficiency at bluer wavelengths. One explanation is that recombination is usually higher when more electrons are injected in the TiO_2 film [16], [17]; with PANI acting as direct electron donor or hole-transporter by being directly attached to the TiO_2/DC hybrid, the recombination process is diminished, and the photocurrents increase due to the electron sequence represented in Scheme 2. Other groups have deposited polyaniline polymers onto TiO_2 and observed sensitization of the semiconductor, that is, under illumination the polyaniline acts as electron donor to the TiO_2 [11], [12]. In our experiments, the change in energetics caused by the presence of the charge-transfer complex might explain why the polyaniline is not able to act as sensitizer and behaves only as secondary electron donor. Nevertheless, because of the relatively high photocurrent production efficiency of the TiO_2/DC hybrid throughout the visible range, our approach of having a secondary electron donor (PANI) directly linked to the TiO_2/DC hybrid yields an improvement in the overall charge-separation process. These processes can be observed in the rise of current as light irradiation hits the films.

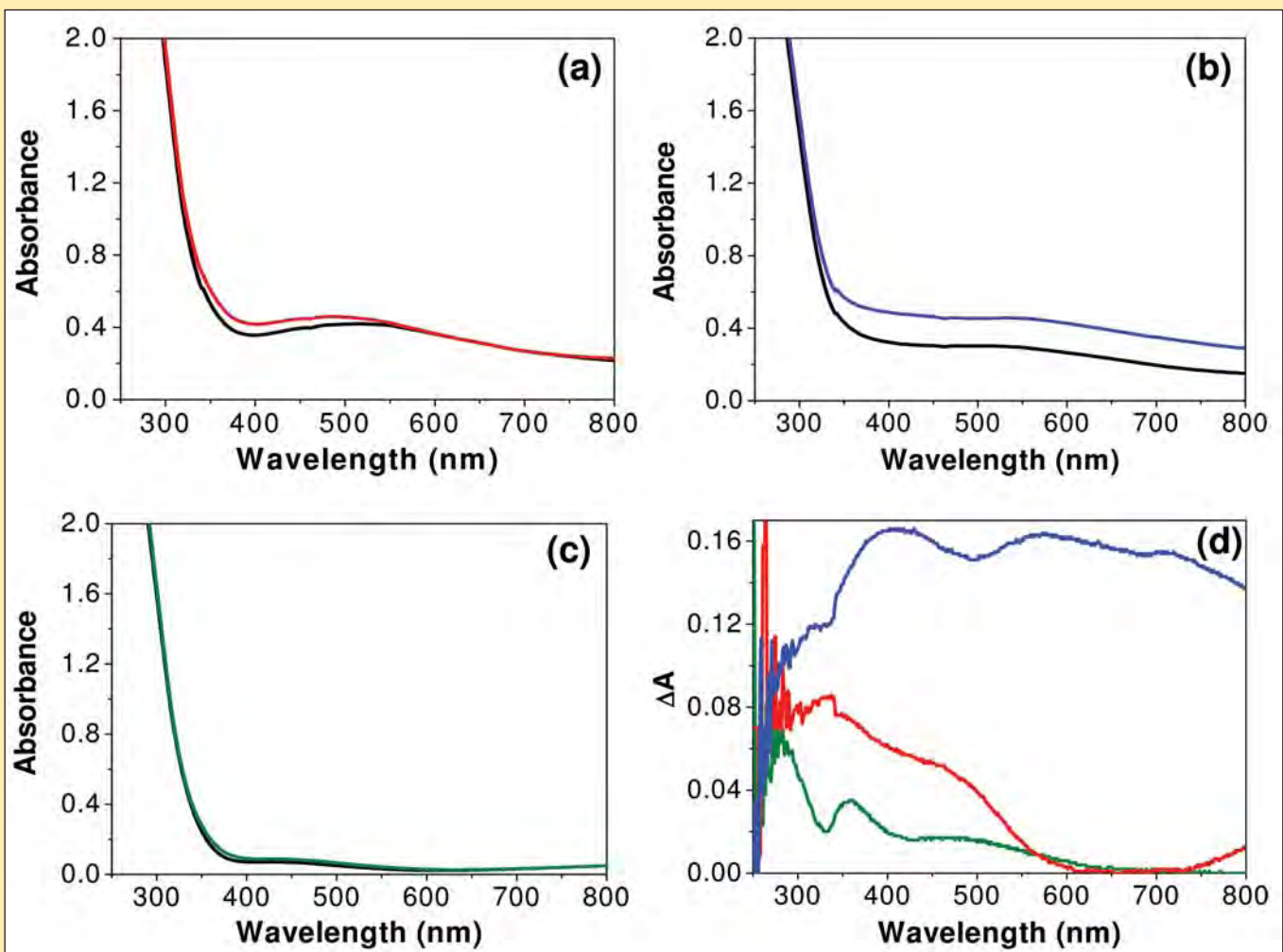


Figure 5. Absorbance spectra of TiO₂ films before and after surface modification: (a) TiO₂/DC (red line), (b) TiO₂/DC/PANI (blue line), (c) TiO₂ soaked in DMF/H₂O solution as control (green line), (d) absorbance differences after minus before modification for a, b and c.

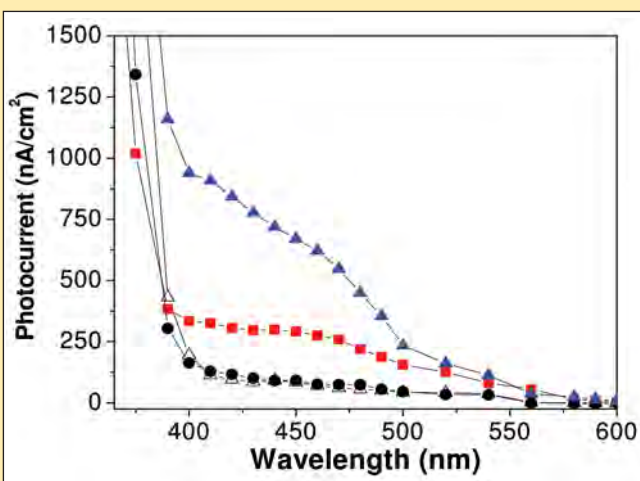


Figure 6. Photocurrent action spectra of TiO₂ electrodes (before modification open triangles), TiO₂ control (filled circles), TiO₂/DC (filled squares) and TiO₂/DC/PANI (filled triangles).

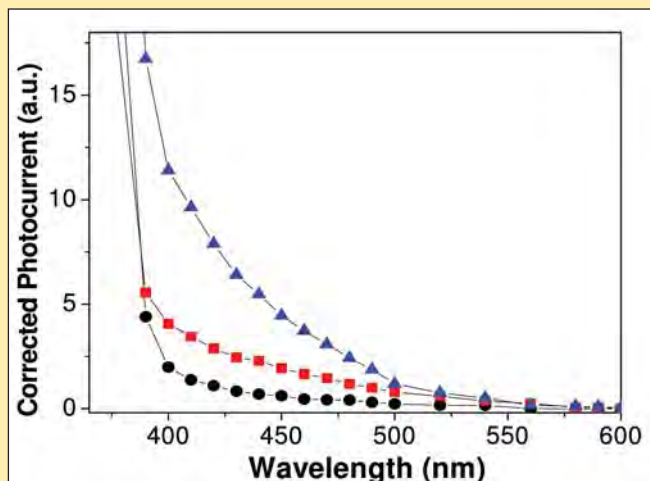


Figure 7. Corrected photocurrent action spectra of TiO₂ control (circles), TiO₂/DC (squares) and TiO₂/DC/PANI (triangles) electrodes. Lamp power at 400 nm was 25 mW/cm².

Collected electrons are measured as current during light-dark cycles obtained as squared-shaped signals during the light cycles at different wavelengths of absorbed light. In Figure 8, current cycles during illumination at 400 nm are shown.

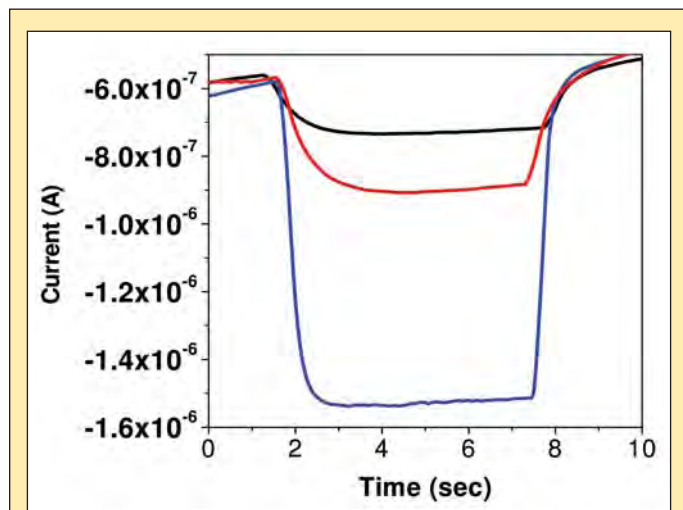


Figure 8. Current curves measured at 400 nm (lamp power was 25 mW/cm²) for TiO₂ (black line), TiO₂/DC (red line) and TiO₂/DC/PANI (blue line) electrodes in dark-light cycles with 5 mM hydroquinone redox donor present in the aqueous electrolyte solution.

The red line shows the dark-light-dark cycle for an electrode modified with DOPAC and the blue line corresponds to an electrode modified with DOPAC-PANI. A blank electrode was soaked in solvent (1:1 DMF/H₂O) as a control. For the TiO₂/DC/PANI films, photocurrent production was higher during illumination of light at 400 nm as compared to TiO₂/DC and the control films. For TiO₂/DC/PANI electrodes, the increase in photocurrent is an end result of sequential electron transfer from PANI to DC preventing charge recombination. For the blank electrode, the photocurrents remain unchanged from that of other unmodified TiO₂ electrodes. In order to compare the shape of the current cycles, normalization was done by dividing each curve by its maximum value. Normalization of current curves shows the rise of current as illumination at 400 nm starts for the three modified electrodes shown in Figure 9.

The blank TiO₂ and the TiO₂/DC electrodes both show a slower rise in photocurrent than the TiO₂/DC/PANI electrode, indicating a higher competition between electron injection and electron recombination. Thus, in the TiO₂/DC/PANI electrode, having the secondary electron directly attached decreases recombination and maintains a more stable photocurrent production. The fast rise in photocurrent shows an efficient charge separation in the modified film along with good electron donation from redox relay (hydroquinone) in solution.

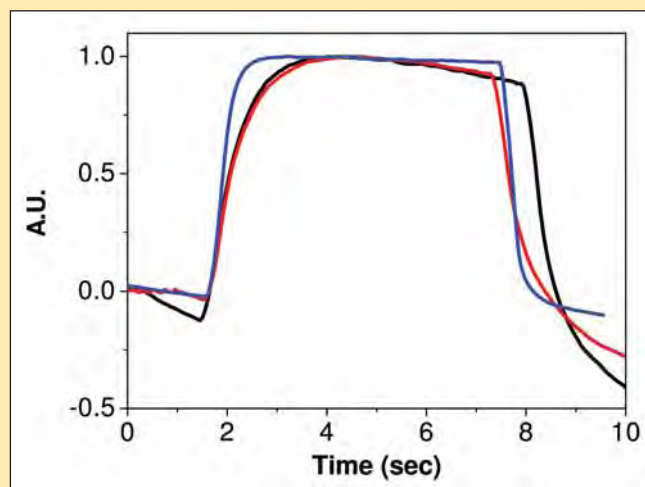


Figure 9. Normalized current curves at 400 nm of TiO₂ control (black line), TiO₂/DC (red line) and TiO₂/DC/PANI (blue line) electrodes in dark-light cycles with 5 mM hydroquinone redox donor present in the aqueous electrolyte solution.

CONCLUSION

The surface properties of TiO₂-modified electrodes were studied using photoelectrochemistry. Significant changes in nanoparticle properties were found for all modified electrodes. Semiconductor triads from TiO₂/DC/PANI formed charge-transfer complexes that produced higher and more stable photocurrents than TiO₂/DC and unmodified TiO₂. The linking of the conductive polymer to the TiO₂/DC greatly increases the photocurrent production in the photoelectrochemical experiments due to a sequential electron transfer from the PANI to the DC ligand. Future work will involve adding another layer of conductive polymer to the TiO₂/DC/PANI films to construct a complete solid-state solar cell.

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IMPROVEMENTS TO THE TIME STEPPING ALGORITHM OF RELAP5-3D

RILEY CUMBERLAND AND GEORGE MESINA

ABSTRACT

The RELAP5-3D time step method is used to perform thermo-hydraulic and neutronic simulations of nuclear reactors and other devices. It discretizes time and space by numerically solving several differential equations. Previously, time step size was controlled by halving or doubling the size of a previous time step. This process caused the code to run slower than it potentially could. In this research project, the RELAP5-3D time step method was modified to allow a new method of changing time steps to improve execution speed and to control error. The new RELAP5-3D time step method being studied involves making the time step proportional to the material courant limit (MCL), while insuring that the time step does not increase by more than a factor of two between advancements. As before, if a step fails or mass error is excessive, the time step is cut in half. To examine performance of the new method, a measure of run time and a measure of error were plotted against a changing MCL proportionality constant (m) in seven test cases. The removal of the upper time step limit produced a small increase in error, but a large decrease in execution time. The best value of m was found to be 0.9. The new algorithm is capable of producing a significant increase in execution speed, with a relatively small increase in mass error. The improvements made are now under consideration for inclusion as a special option in the RELAP5-3D production code.

INTRODUCTION

Time stepping is an important component of numerical models. Choosing the appropriate time step is necessary to minimize both the execution time of the code and the error of the model. The purpose of this research project is to study the usage of a time step that is proportional to the material courant limit (MCL) of the model, and to consider this method of time step selection as a possible improvement to RELAP5-3D/Version 2.4.1.2 [1].

RELAP5 is a reactor multiphysics code that models both neutronics and thermo-hydraulics. It is used by engineers around the world to model these phenomena. Additionally, it is used at reactor facilities in the United States to run accident scenarios in training simulations. It was created at the Idaho National Laboratory (INL).

The code employs several mathematical models. For the fluids of the reactor, it uses a finite difference approximation to solve the six equation model of two-phase fluid flow. This model consists of a set of six partial differential governing equations that describe: liquid mass, vapor mass, liquid momentum, vapor momentum, liquid energy, and vapor energy. Appropriate closure relations are used to solve for additional variables. The code uses a finite difference method for multi-dimensional heat transfer equations and an analytical nodal method for neutron kinetics. Both semi-implicit and “nearly-implicit” finite difference time stepping schemes are available [1]. The focus of this work is on the former scheme, semi-implicit. Additionally, RELAP5 has models for both plant trips and controls [1]. It is used in reactor design, licensing and operator training simulators.

The time step in RELAP5 is constrained by numerous conditions; namely user input, code stability and code error control. The user input includes the maximum and minimum time step sizes, the frequency of plots, printed output, restart record dumps and optional error control specifications. The semi-implicit time step method keeps the time step below the MCL for code stability. To control mass error, the time step is adjusted to keep the error of each advancement sufficiently small. In the current version, if error or stability conditions are not met, the time step is cut in half. If the conditions are met extremely well, the time step is doubled [1].

For the best code execution time, the time step ideally should be just below the MCL. However, the time step may never exceed the user-supplied maximum step size, which can be far below the MCL. Even when MCL is below the maximum step size, the halving/doubling scheme can select a time step nearly half the size of the MCL. It is thus necessary to replace both of these constraints on time step size in order to approach the ideal time step size.

All of the functions previously described for time step control in RELAP5 are computed in subroutine DTSTEP. The subroutine is responsible for numerous other functions including determining when to create output, terminate a transient and communicate via the parallel virtual machine with other codes [1].

As the goal of this research project is to improve code efficiency, i.e., reduce RELAP5 run time without compromising code accuracy, several alternate time step algorithms are developed and implemented. Measures of the code performance are explained and presented.

METHODS

Description of Original Time Stepping Method

The MCL is an important constraint for calculating time steps for the semi-implicit time advancement method in RELAP5-3D. It is computed for volume i according to Carlson [1] as shown below.

$$\Delta t_i^n = \Delta x_i \frac{\max(\alpha_{fi}^n, \alpha_{gi}^n)}{\max(|v_{fi}^n \alpha_{fi}^n|, |v_{gi}^n \alpha_{gi}^n|)} \quad (1)$$

Here Δx_i is the characteristic length dimension of the control volume. v is the velocity of the fluid. α is the void fraction. Subscript f indicates a liquid phasic property. Subscript g indicates a gaseous phasic property. Superscript n is the time advancement number. Δt_i^n represents the time it takes for fluid entering at one boundary of control volume i to cross to its exit boundary during time advancement n . The MCL for the entire flow region is given by: [1]

$$MCL = \min\{\Delta t_i^n | i = 1, \dots, NVOL\} \quad (2)$$

where NVOL is the number of control volumes in the flow region. This ensures that no control fluid crosses more than one control volume in a single advancement. With the semi-implicit time stepping method, this is the stability limit since steps larger than this can cause instabilities.

Despite the possibility of instability and in order to take larger time steps, DTSTEP does not strictly enforce the MCL condition, $\Delta t < MCL$. Rather, it sorts the control volume Δt_i^n into five groups based on the control volume number. Thus, group 1 would contain volumes 1, 6, and 11 and group 2 would contain volumes 2, 7, and 12, etc. The smallest minimum of any group is denoted MCL_1 , the second smallest group minimum, MCL_2 , etc. Note that $MCL_1 = MCL$ in the above condition. By default, MCL_2

is selected as the MCL for time stepping. The user can select to enforce equation (2) by turning on card 1, option 15. Either way, the MCL condition in the original halving/doubling algorithm is given by Carlson [1].

$$\Delta t = \max\left\{\frac{DTMAX}{2^k} \mid \frac{DTMAX}{2^k} < MCL_j, k=1,2,\dots\right\}, j \in \{1,2\} \quad (3)$$

Equations (1), (2) and (3) form the original algorithm, denoted A1. Because of (3), Δt is rarely larger than the actual MCL of equation (2). There are occasions, however, when $\Delta t > MCL$. In this project we study and implement methods that allow larger Δt while always satisfying equation (2).

Another time step constraint is the fact that edit times (plot, major edit, and restart times) must be reached exactly. To accomplish this, the number of advancements needed to reach the next integer multiple of DTMAX is stored in the integer variable NREPET, an integer giving the number of permutations (all edit times are multiples of DTMAX). For example, if the current time step is $0.25 \cdot DTMAX$, and the cumulative time is $5.25 \cdot DTMAX$, then NREPET equals three. This is because three more time steps of the current size are needed to reach the next integer multiple of DTMAX; namely $6 \cdot DTMAX$. When the time step is halved, NREPET is doubled, and when the time step is doubled, NREPET is halved.

As a result of truncation due to integer division, the time step can only be doubled when NREPET is even which causes inefficiency. In the previous example, doubling when $\Delta t = DTMAX/4$ is not allowed because the truncation of $3/2$ to 1 would indicate that only one step of size $DTMAX/2$ is needed to reach from $5.25 \cdot DTMAX$ to $6 \cdot DTMAX$. Thus, the use of NREPET causes the code to take more advancements than necessary to reach the end time of the transient. To increase code efficiency, NREPET should be replaced.

NREPET has two uses: to control time step size and to help determine when edits are necessary. When odd, NREPET prevents the time step from being doubled. An NREPET equal to zero indicates that current time is a multiple of DTMAX. For the NREPET system to work properly (allowing for the time step to hit time targets) the time step must increase and decrease by the same factor. If this is not the case, the time step will cease to hit time targets due to round-off error which prevents the time step size from approaching the MCL. Therefore, replacing the NREPET with an MCL-based time step control is a natural objective. The second purpose of NREPET is to help check if an edit needs to be performed since edits are only performed when NREPET = 0.

The original version of DTSTEP implements time step control with floating point data. For accuracy, these are being replaced by an equivalent method of time tracking based on integer data. This allows NREPET, an integer variable, to be replaced naturally by the integer timekeeping data of the new integer algorithm.

Implementation of the New Method

The integer version of subroutine DTSTEP/Version 2.4.1.2 implements 11 major functions as 18 major sections and sub-sections. Jumps within sub-sections and between sections make the code difficult to read and modify. Therefore, to improve readability at the outset, 18 FORTRAN 90 internal subroutines were separated out of the original DTSTEP code. This reduced the amount of

executable code in the main DTSTEP subroutine from an original 1 400 lines to only 350 lines; making the code much easier to read.

Two functions of NREPET, control of halving/doubling and determination of whether the current time is a multiple of DTMAX, were implemented using an equivalent variable from the integer time algorithm. The time step control algorithm was then modified to use MCL to determine increased time step size. Time step halving, however, was continued in order to control error. The modified algorithm, A2, is:

$$\left\{ \begin{array}{l} \Delta t = \Delta t / 2, \\ \Delta t = \min(2\Delta t, m \cdot MCL_1, DTMAX), \end{array} \right. \begin{array}{l} \text{if MCL stability or error condition, or} \\ \text{3 successive, non-ideal advancements,} \\ \text{if mass error condition allows increase} \end{array} \quad (A2)$$

here, $0 < m < 1.0$. The removal of NREPET allows the time step to be set to any value as long as targets continue to be hit and the model remains stable.

Coding for algorithm A2 was placed at the end of DTSTEP rather than scattered throughout. This created implementation issues. For example, when conditions requiring a time step halving were met, a logical variable recorded it and it was used in the if-section of A2. During testing, it was discovered that implementing A2 at the end could cause indefinite repeating of the same time step. This was overcome by specifying that the time step would again be halved if there were three unsuccessful advancements in a row.

To more closely approach MCL, a violation of DTMAX was necessary; leading to algorithm A3. For input models with no flow conditions, MCL is essentially infinite. Algorithm A3 employs an upper limit, arbitrarily selected as 20-DTMAX, to prevent this.

$$\left\{ \begin{array}{l} \Delta t = \Delta t / 2, \\ \Delta t = \min(2\Delta t, m \cdot MCL_1), \\ \Delta t = \min(2\Delta t, m \cdot MCL_1, DTMAX), \end{array} \right. \begin{array}{l} \text{if MCL unstable or error condition, or} \\ \text{3 successive, non-ideal advancements,} \\ \text{if mass error condition allows increase,} \\ \text{and MCL} > 10^6 \text{ seconds.} \end{array} \quad (A3)$$

The elimination of NREPET created a DTSTEP output problem with algorithms A2 and A3. Since MCL is unpredictable, seldom did cumulative time ever match edit time. D_n , the difference between edit time and cumulative time, divided by three is compared with the time step. If $\Delta t^n \leq D_n$, three steps of nearly equal size are taken to reach the time target. The first step may be slightly larger due to aspects of the integer algorithm beyond the scope of this report, but the final two are equal. This is summarized in algorithm A4.

$$\left\{ \begin{array}{l} \Delta t = \frac{t_{edit} - t}{3} + \text{mod}(t_{edit} - t, 3), \text{ Three remaining steps.} \\ \Delta t = \frac{t_{edit} - t}{2}, \text{ Two remaining steps.} \\ \Delta t = t_{edit} - t, \text{ One remaining step.} \\ \Delta t = t_{saved} + \text{Time target reached.} \end{array} \right. \quad (A4)$$

In some transients, conditions required a time step reduction by a factor of two during the A4 process. In those cases, the time targeting process, A4, was deactivated until the time target was again within three current time steps of the current time.

Performance Measurements

Four sets of combined algorithms, C_1 – C_4 , were tested with several input models. The input models or test cases, are combinations of hydrodynamic components, heat structures, plant controls, initial conditions and boundary conditions. The combined

algorithms consist of various combinations of the MCL following algorithms (A2 and A3) with the time targeting algorithm (A4). An additional distinction between the combined algorithms was whether MCL_1 or MCL_2 was being used. These combined algorithms are summarized in Table 1.

Combined Algorithm Description	DTMAX condition	Courant Control
C_1 , A2 with A4	enforced	$m \cdot MCL_2$
C_2 , A3 with A4	ignored	$m \cdot MCL_2$
C_3 , A2 with A4 and Option 15	enforced	$m \cdot MCL_1$
C_4 , A3 with A4 and Option 15	ignored	$m \cdot MCL_1$

Table 1. Description and comparison of the algorithms.

To examine the workings of the new algorithms, time step size and MCL_1 were recorded throughout two runs of TYP12002, one with DTMAX imposed and one with it ignored. MCL_2 was used to control the time step. The code, by default, outputs MCL_1 even when MCL_2 is in use.

Additionally, a comparison of the four algorithm combinations was made by varying m between 0.4 and 1.2 by steps of 0.05. With each variation of m , the test cases were executed five times. Measures of mass error and execution speed were recorded with each run. The recorded run times were adjusted to not include input processing time which will be constant for each model. The test cases run were: ANS79, CTEST1, FWHTR, NC, NEPTUNUS20, SCW, and TYP12002. Brief descriptions can be found in Table 2. For more detail of these test cases, refer to Carlson [2]. This variety of test cases is intended to expose any trouble that might occur with the new algorithms, as well as to show that the new algorithm is an improvement in most cases. As a whole, they represent the range of operating conditions that the new algorithm might encounter. This is the case with the notable exception of the parallel virtual machine, which is beyond the scope of this research project.

Model	Description
ANS79	Two volume pipe; tests long term decay heat study
CTEST1	Two loop plant with steam generator, nuclear core, pump and pressurizer
FWHTR	RELAP5-3D feedwater heater component model test
NC	Water/steam-filled piping network test of five separate cases of non-condensable gases: Air, CO, CO ₂ , O ₂
NEPTUNUS	NEPTUNUS pressurizer test y05
SCW	Reactor vessel model run to steady-state testing of the supercritical water of properties
TYP12002	Typical Pressurized Water Reactor; 1200 second transient

Table 2. Brief descriptions of each model used [2].

As a control, each test case was run twice, first with MCL_1 and then with MCL_2 , using the original integer algorithm. Measures of mass error and execution speed were recorded with each run. Central processing unit (CPU) times were, however, not recorded due to the findings from the measurements previously described.

Two different measures of mass error were employed. Cumulative mass error is too sensitive to small changes in the timing of events to provide an effective measure of performance; therefore

two other measures were developed. These are shown in equations (4) and (5):

$$\text{Integral of Mass Error} = \frac{1}{\text{Execution Time}} \int (\text{Cumulative Mass Error}) dt \quad (4)$$

The absolute mass error rate is the average amount of mass that either appears or disappears from the numerical model per unit time. It is calculated with the formula:

$$\text{Absolute Mass Error Rate} = \frac{1}{\text{Execution Time}} \int \left| \frac{d(\text{Cumulative Mass Error})}{dt} \right| dt \quad (5)$$

The latter equation sums the mass appearing and disappearing in the system due to truncation. The cumulative mass error rate however, sums up mass error without regard to whether it appears or disappears. If mass disappears and then reappears, then cumulative mass error will be zero, but error will still exist in the rest of the solution. The absolute mass error rate measure circumvents this and treats all mass error as a positive quantity. This produces another measure of accuracy similar to the cumulative mass error rate. This rate allows comparison of test cases with different execution times.

RESULTS

The results show a significant improvement in execution time when the time step is unbounded by DTMAX, using algorithm combinations C_2 and C_4 . There is also occasional improvement with algorithm combinations C_1 and C_3 , where DTMAX is enforced. It is also found that algorithm combinations C_1 – C_4 work best with m set to 0.9.

Figure 1 shows two graphs of MCL vs. time for algorithms C_1 and C_2 running the TYP12002 model with m at 0.9. This test case is very sensitive to time step selection, because of the model's layout. For C_1 , the time step remains constant well below the MCL with some reductions due to excessive mass error as seen in Figure 1.

For C_2 , the time step remains slightly below MCL. At about 0.33 seconds, it levels out at one third of the time between edits and is 3.3 times as large as the time step size in the C_1 algorithm where DTMAX is imposed. This can also be seen in Figure 1. Despite the fact that only the time step size changed, the MCL varies quite substantially between graphs A and B in Figure 1. Similar behavior occurs in TYP12002 with the original integer-time coding running below DTMAX.

It was found that in all input models, the number of advancements was proportional to the run time as shown in Figure 2.

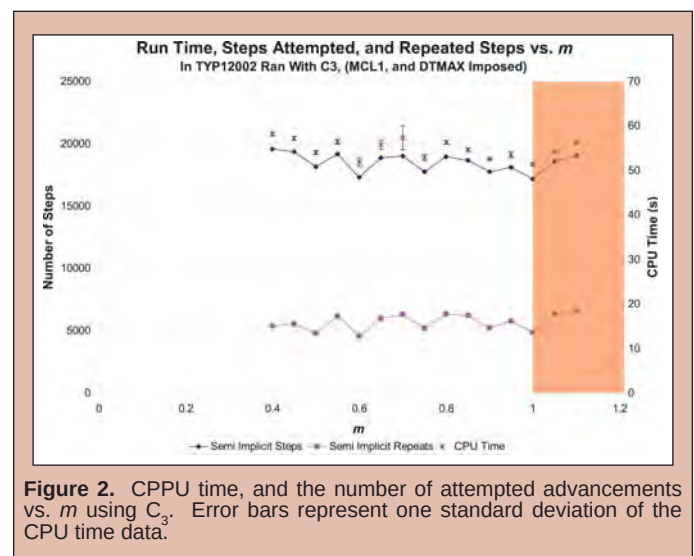


Figure 2. CPU time, and the number of attempted advancements vs. m using C_3 . Error bars represent one standard deviation of the CPU time data.

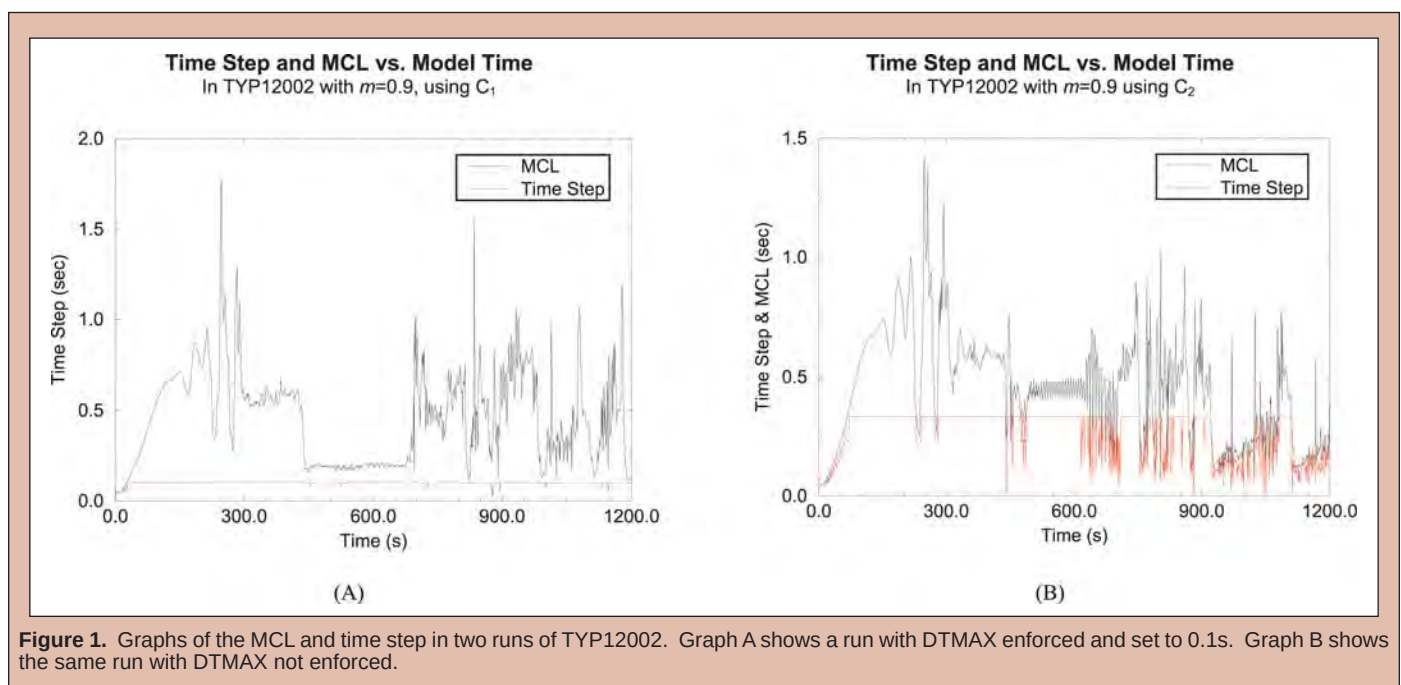


Figure 1. Graphs of the MCL and time step in two runs of TYP12002. Graph A shows a run with DTMAX enforced and set to 0.1s. Graph B shows the same run with DTMAX not enforced.

Response to Changing m

The test cases had three types of response to a changing m : constant, smooth, and chaotic.

Constant Category

In four of the seven test cases, ANS79, FWHTR, NEPTUNUS20 and SCW the number of advancements is unaffected by changes to m . This is named the “constant” category. Also, changing between MCL_1 and MCL_2 has very little effect on the results. Further, algorithm combinations C_1 and C_3 , with DTMAX imposed, take approximately the same number of steps as integer-time DTSTEP, Version 2.4.1.2/Interim Version r5b. However, algorithm combinations C_2 and C_4 , which ignore DTMAX, greatly reduce the number of attempted advancements for these tests. As seen in Figure 3, the number of steps is often reduced by about 80%.

Smooth Category

Two cases, CTEST1 and NC, comprise the smooth category. These are by far the most notable. The run of CTEST1 best represents the smooth category. Consider Figure 4, graph A. On the right side, the curves for C_1 and C_3 (DTMAX enforced) converge. On the left, curves for C_1 and C_2 (using MCL_2) converge, as do C_3 and C_4 (using MCL_1).

The mass error rate in this category was not as stable as that in the constant category. The curves with DTMAX enforced (C_1 and C_3) still converge at the left side, while the others do not. Also, when m approaches the courant limit, mass error gets very large. This happens with m equal to 1 when MCL_1 is used. Additionally, the removal of DTMAX, caused an increase in the absolute mass error rate as seen in Figure 4, graph B.

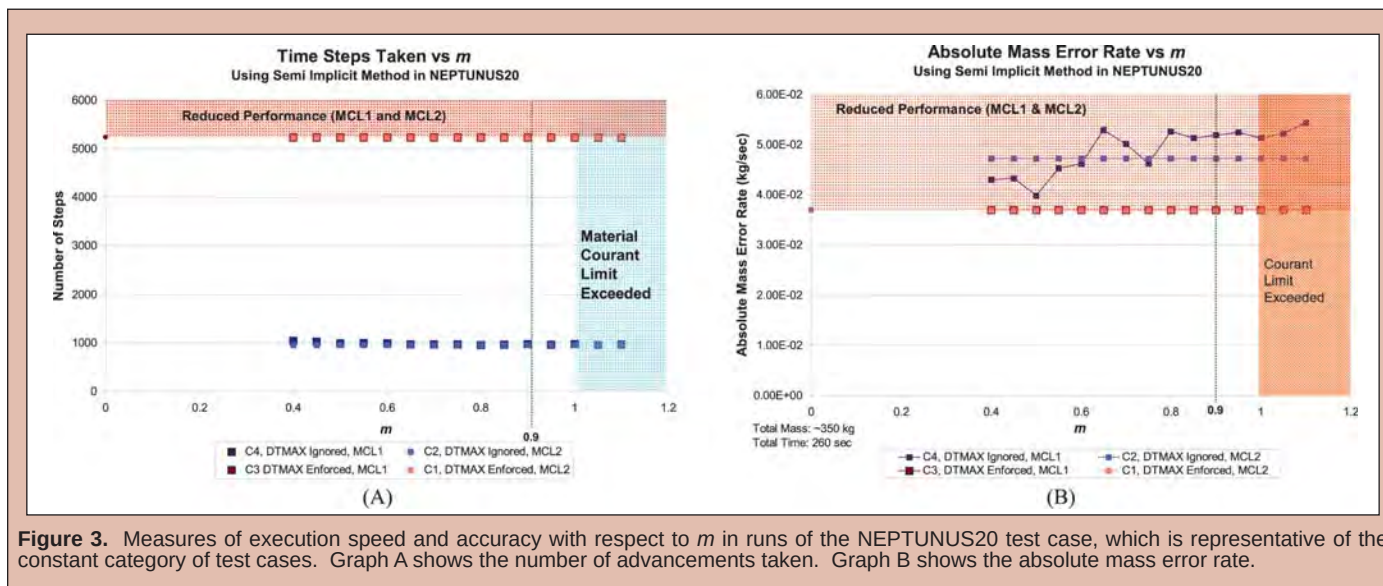


Figure 3. Measures of execution speed and accuracy with respect to m in runs of the NEPTUNUS20 test case, which is representative of the constant category of test cases. Graph A shows the number of advancements taken. Graph B shows the absolute mass error rate.

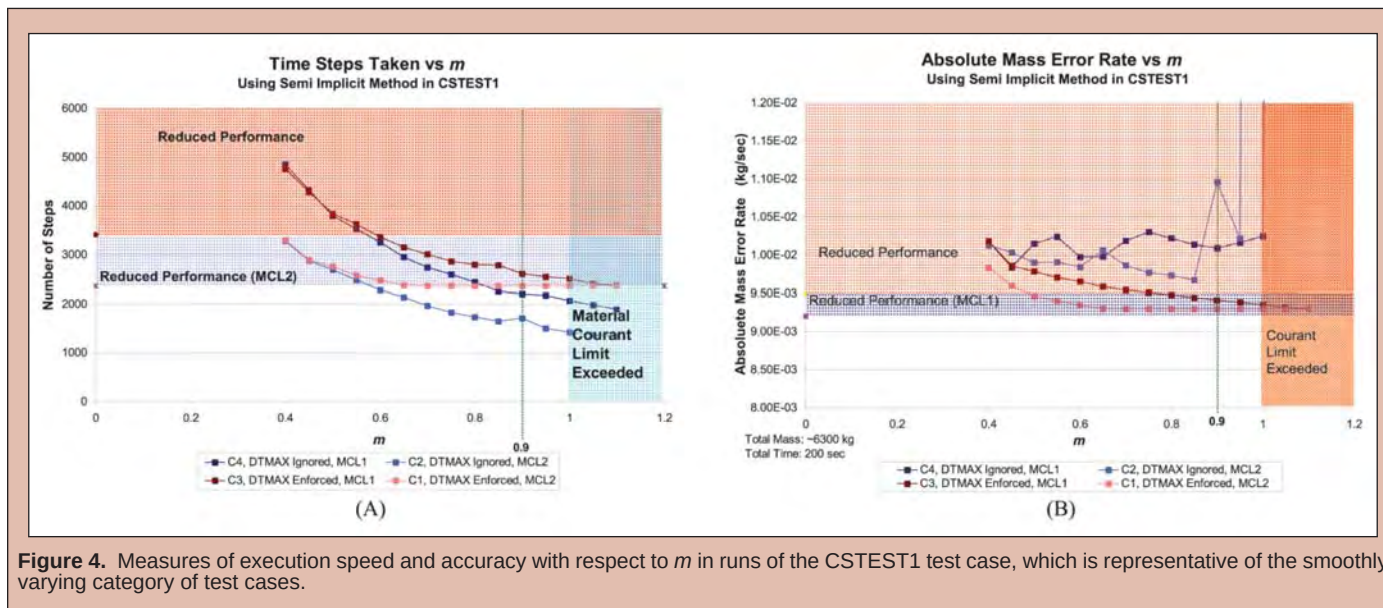


Figure 4. Measures of execution speed and accuracy with respect to m in runs of the CTEST1 test case, which is representative of the smoothly varying category of test cases.

Chaotic Category

Only one test case, TYP12002, responded noisily to a changing m . This can be seen in Figure 5. The numbers of advancements attempted are grouped according to whether DTMAX is imposed or not. The curves without DTMAX imposed decrease slightly with increasing m . These curves also contain some noise. This can be seen in Figure 5, graph A. Figure 5, graph B shows that the mass error also behaves chaotically.

DISCUSSION AND CONCLUSION

Figures 3 through 5 show that the value of 0.9 is an acceptable value for m for virtually all input models. For some input models, failures occur at $m = 1.0$ and for others, failures occur at smaller values. However, 0.9 is always shown to be safe. The value $m = 0.9$ is recommended as it generally produces the best results as well.

The results show that it is possible to greatly increase the execution speed of RELAP5 by using algorithms C_2 and C_4 (which ignore DTMAX), while producing only a relatively small increase in the mass error rate. This is especially true in the smooth test cases where the number of attempted advancements is decreased by 80%, while the absolute mass error rate increased no more than 30%. This is often the same as in the DTSTEP/Version 2.4.1.2/Interim Version r5b. Since mass error is already so small relative to the massive amounts of fluid in the systems, this 30% increase should be acceptable to most users.

The smooth test cases show the relation between the competing forces of DTMAX and the MCL in the time step selection. As was seen in the results section by the convergence on the left; when m is small, the MCL determines behavior. As was seen by the convergence on the right; when m is large, DTMAX determines behavior. Thus, the larger m loosens the MCL constraint.

It is conceivable that the rate of edits caused the constant curves to not change with m . Because of the way the new edit time targeting algorithm A4 works, the time step can never exceed one third of the time between edits. This is seen somewhat in Figure 1, graph B), although that test case is chaotic. If the MCL is always

larger than the time step imposed by the edit frequency, the curve will not depend on m .

By reviewing Figures 3 through 5, it can be seen that algorithm C_4 with MCL₁ and DTMAX ignored is generally the best for reducing the number of advancements, and thereby increases the code run speed the most. This is because it never violates equation (2) and therefore, it always remains stable. It also allows the time step to approach the ideal time step size of the MCL.

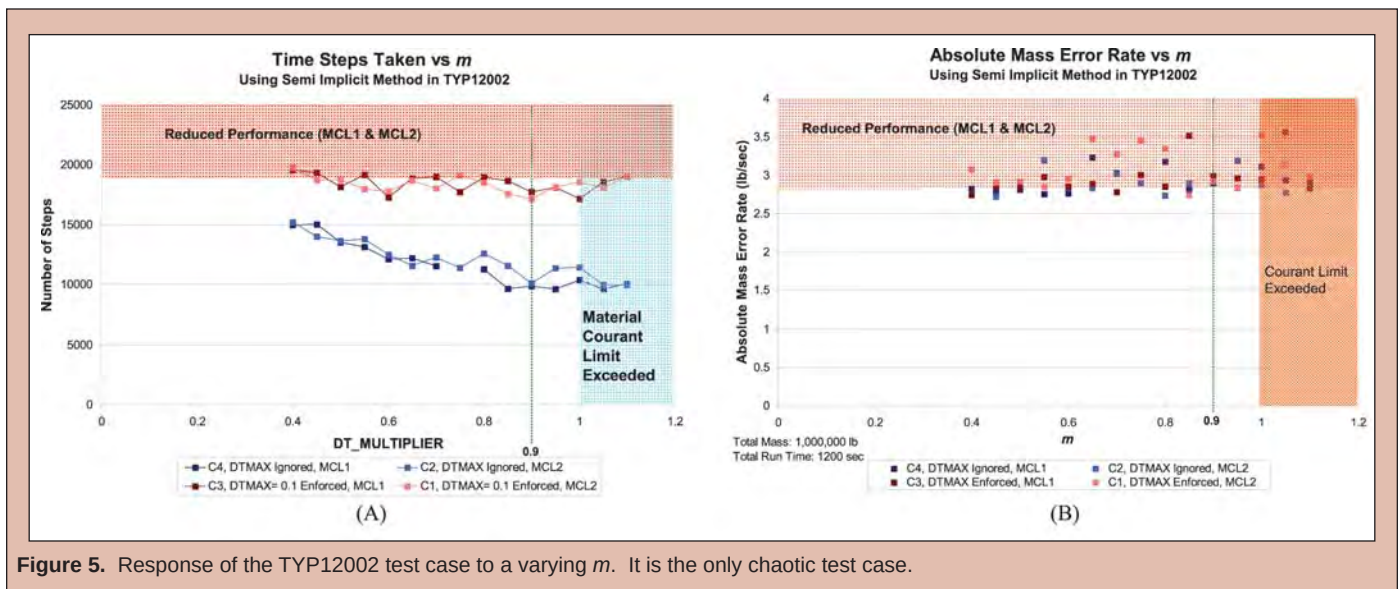
The final conclusion of this study is that algorithm C_4 , which strictly imposes the MCL condition of equation (2) and ignores DTMAX, with $m = 0.9$, produces the best results for most of the test cases. It reduces the number of advancements and code run time by up to 80%, while increasing measures of mass error by no more than 30%. Algorithm C_4 should be implemented in RELAP5-3D as a permanent user option.

ACKNOWLEDGMENTS

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MODELING WIND TURBINES IN THE GRIDLAB-D SOFTWARE ENVIRONMENT

JASON C. FULLER AND KEVIN P. SCHNEIDER

ABSTRACT

In recent years, the rapid expansion of wind power has resulted in a need to more accurately model the effects of wind penetration on the electricity infrastructure. GridLAB-D is a new simulation environment developed for the U.S. Department of Energy (DOE) by the Pacific Northwest National Laboratory (PNNL), in cooperation with academic and industrial partners. GridLAB-D was originally written and designed to help integrate end-use smart grid technologies, and it is currently being expanded to include a number of other technologies, including distributed energy resources (DER). The specific goal of this project is to create a preliminary wind turbine generator (WTG) model for integration into GridLAB-D. As wind power penetration increases, models are needed to accurately study the effects of increased penetration; this project is a beginning step at examining these effects within the GridLAB-D environment. Aerodynamic, mechanical and electrical power models were designed to simulate the process by which mechanical power is extracted by a wind turbine and converted into electrical energy. The process was modeled using historic atmospheric data, collected over a period of 30 years as the primary energy input. This input was then combined with preliminary models for synchronous and induction generators. Additionally, basic control methods were implemented, using either constant power factor or constant power modes. The model was then compiled into the GridLAB-D simulation environment, and the power outputs were compared against manufacturers' data and then a variation of the IEEE 4 node test feeder was used to examine the model's behavior. Results showed the designs were sufficient for a prototype model and provided output power similar to the available manufacturers' data. The prototype model is designed as a template for the creation of new modules, with turbine-specific parameters to be added by the user.

INTRODUCTION

In recent years, the use of wind generated power, as both a centralized source of power (such as wind farms) and as a distributed resource, has rapidly increased. As wind power penetration increases, the negative effects upon the transmission and distribution systems can no longer be ignored; they must be modeled and examined in further detail [1], [2], [3]. Additionally, recently developed technologies, including Grid-Friendly™ appliances and other distributed energy resources (DERs) are being incorporated into existing power systems and by extension, into existing and newly developed software simulation environments. The effects of these new technologies become particularly important as more of these technologies are deployed within the electricity infrastructure. The goal of this project is to develop a preliminary wind turbine generator (WTG) model to be incorporated into one of these new software systems, GridLAB-D.

GridLAB-D is a new simulation system developed for the U.S. Department of Energy (DOE) by the Pacific Northwest National Laboratory (PNNL) in collaboration with industrial and academic partners. GridLAB-D is a unique simulation environment, in that it is a generalized simulation environment that is specifically designed to be used with multiple processors. Based on the architecture of GridLAB-D, the transmission power flow solution technique implements the Gauss-Seidel method [4], while the distribution power flow technique is implemented with the forward and backward sweep (FBS) method. GridLAB-D finds quasi-steady state time series solutions that, when put together, approximate the time-varying, non-dynamic solution. The FBS method is described by Kersting [5], and further information and description of the software's capabilities, and the reasons behind its creation, are provided by the designers [6]. DOE initiated this software with the intent to eventually release it as open-source software to facilitate

the analysis of smart grid technologies, with the idea that developers can create, test and connect their own individual modules. The modules can represent a wide variety of components, from end-use products (refrigerators or light bulbs) to generation equipment (wind turbines or solar cells), as well as transmission components (transformers or relays).

Since GridLAB-D is designed as a modular simulation environment, the incorporation of new generator components involves the creation of new modules to represent the generators; modification of other existing modules is not necessary. It is up to the user to determine the level of detail that any such module will incorporate. The prototype WTG model created in this project breaks the wind turbine down into its basic components which are modeled individually. A simple layout of major WTG components includes a three-blade rotor attached to a drive shaft which in turn drives a generator, typically through a multi-stage gear box. Depending on the type, location and application, some wind turbines are directly coupled to local electricity infrastructure, while others are filtered through inverter/rectifier combinations, shunt capacitors, or other power electronics and controlled by feedback systems. Figure 1 shows a simple schematic of a WTG used in conjunction with power electronics. This project developed the prototype WTG model up to, but not including, controls and power electronics.

METHODS

Modeling characteristics of the WTG can be divided into two main categories; mechanical power produced by the wind and electrical power converted from the mechanical power. The models used in this project are broken into these two constituent parts.

Mechanical Power

GridLAB-D uses meteorological data supplied by the National Renewable Energy Laboratory (NREL) in the Typical Meteorological Year format (TMY2) to provide input data for individual WTGs. The TMY2 format includes hourly meteorological data, such as wind speed, air temperature and elevation, from 239 stations across the United States for a 30 year period (1961–1990) [7]. In GridLAB-D, meteorological data can be imported into individual modules and used to simulate a time series solution with steady state steps.

As wind passes across the turbine blades, the kinetic energy is converted into mechanical power. According to Betz' law, a maximum of 59% of this power can be extracted [8]. However, actual applications are typically less efficient than this. The power extracted from the wind by the turbine can be expressed as

$$P_m = P_{wind} \times C_p(\lambda, \beta), \quad (1)$$

where P_m is the mechanical power extracted by the turbine blades and $C_p(\lambda, \beta)$ is the coefficient of performance, or the fraction of power that is extracted from the wind. The tip speed ratio, λ , is the ratio between the turbine blade tip speed and the wind speed, and the pitch angle, β , is the angle of attack of turbine blades. Only a few manufacturers openly supply tables that give the coefficient of performance for any given integer wind speeds. In the cases where a manufacturer's table was available, a tenth order polynomial interpolation function was generated in Matlab to give a continuous function to estimate the manufacturer's data at all wind speeds. In cases where performance data was not available, the method described by Justus [9] was used.

According to Justus, and further explained by Malinga [3], at any given pitch angle an approximation of performance can be given by

$$C_p = \begin{cases} C_{pm} \times \left[1 - F \left(\frac{u_m}{u} - 1 \right)^2 - G \left(\frac{u_m}{u} - 1 \right)^3 \right], & u_c \leq u \leq u_r \\ C_{pr} \times \left[\frac{u_r}{u} \right]^3, & u_r \leq u \leq u_f. \end{cases} \quad (2)$$

Wind speed, u , determines the coefficient of performance for any given turbine model, and is divided into two distinct regions, below and above rated wind speed, u_r . The cut-in wind speed, u_c , and the cut-out wind speed, u_f , are the boundary values which determine the operating range of the turbine model. C_{pm} and C_{pr} , respectively, are the maximum values of the coefficient of performance and the coefficient of performance value at rated wind speed, while u_m is the wind speed at which the maximum C_{pm} occurs. F and G are coefficients which can be found by applying the boundary conditions. By using manufacturer's data for cut-in, cut-out and

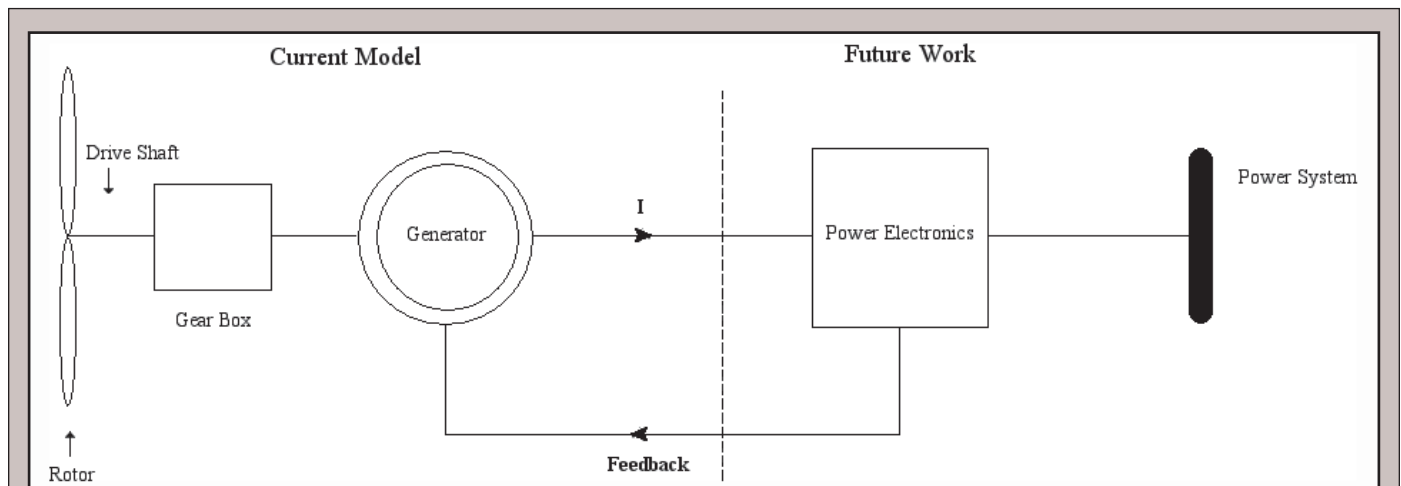


Figure 1. Basic wind turbine configuration.

rated wind speeds and power output at rated speeds, an estimated coefficient of performance function can be generated to approximate the performance of a real turbine. This method only fully applies to fixed pitch turbine systems, where the pitch angle of the blade is constant. In a variable pitch turbine, the blade pitch is adjusted at a given wind speed to gain the highest achievable coefficient of performance value. This means that the Justus model is not entirely accurate for variable pitch turbines at lower wind speeds; however, it is sufficient for the model at this stage of development, and can represent either pitch style, regardless of generator type.

The coefficient of performance gives the percentage of the power that can be extracted from the wind. The total power for extraction available in the wind is given by

$$P_{wind} = \frac{1}{2} \rho A u^3, \quad (3)$$

A is the area swept, πr^2 , by the turbine rotors in meters squared, and ρ is the density of the air passing across the turbine. Air density is affected by atmospheric conditions, such as temperature, pressure and elevation, and can alter the power output by as much as 40% for a given turbine and wind speed. At this time, the climate model within GridLAB-D does not support all the necessary climate components, including air pressure, so air density was calculated assuming constant standard pressure and using imported TMY2 temperature data. Future versions of GridLAB-D will support these features, and functions were put in place to eventually use location-specific data to determine air density.

A certain amount of mechanical power is lost in the drive train gearbox. The blade and hub assembly on a wind turbine will typically spin at 12–18 revolutions per minute, while to deliver AC power at a nominal frequency of 60 Hz, the generator shaft needs to spin at 1 200–1 800 rpms. The gearbox steps up the rotational speed of the shaft but also incurs mechanical losses due to friction. Cotrell [10] shows that a 1% loss of rated power per stage due to viscous friction losses is a reasonable assumption. Aguglia [11] describes the gearbox losses as

$$\eta_{gear} = 1 - q \times 0.01 \times \frac{P_{gear_rated}}{P_{in}}, \quad (4)$$

where q is the number of gearbox stages on the shaft. The total extracted mechanical energy into the generator can now be given as

$$P_m = \frac{1}{2} \rho \pi r^2 C_p(u) \eta_{gear} u^3, \quad (5)$$

Mechanical power extracted can be determined as a function of wind speed and current atmospheric conditions for any given wind turbine.

One final adjustment was made to calculate the extracted power. Most meteorological data is measured at 5 to 15 m height, as is the case with the TMY2 data; however, wind turbines are significantly taller. Wind shear near the ground, which is affected by the roughness of the local terrain, significantly reduces the wind speed at lower levels. A correction factor,

$$u_{adj} = u_{ref} \times \frac{\ln\left(\frac{z}{z_o}\right)}{\ln\left(\frac{z_{ref}}{z_o}\right)}, \quad (6)$$

used by the European Wind Atlas [12], was used to adjust the wind speed as measured at 10 m to approximate the strength of the wind at the height of the wind turbine. The measured wind speed, u_{ref} at height z_{ref} is adjusted to the turbine hub height, z , through the use of a roughness length factor, z_o . The roughness length factor is a unit-less correction factor that approximately describes the amount of wind shear at a given location due to local terrain. For example, over water, $z_o = 0.0002$, while over rough agricultural land, $z_o = 0.4$, and can have a sizeable effect on the amount of power generated at the turbine hub height.

Converted Electrical Power

Mechanical power supplied by the wind is converted to electrical power through a synchronous or induction generator. Permanent magnet synchronous generators (PMSGs) have been the commonly used form in general applications; however, doubly-fed induction generators (DFIGs) have become increasingly popular, as they have the ability to not only absorb reactive power, but they also provide reactive power to assist in voltage stability [13]. DFIGs are essentially induction generators with complex feedback loops that can control the reactive power output of the generator. Since induction generators will always absorb reactive power and cannot provide it, they are not widely used without additional hardware, such as shunt capacitors. DFIGs were created as an alternative to this problem, and are becoming more popular since they are generally cheaper and lighter than corresponding PMSGs. This project began the process of creating a PMSG model with limited control systems, and took the first steps in modeling an induction generator for future use as a DFIG.

Synchronous Generator

The PMSG was modeled using a balanced Y-grounded circuit, but has the capability to be implemented with unbalanced generator parameters. The per-phase model is shown in Figure 2. V_{phase} is the voltage from one terminal to neutral and is determined by the bus line voltage. The circuit is solved through an iterative process, in which the final desired output is the current supplied to the grid,

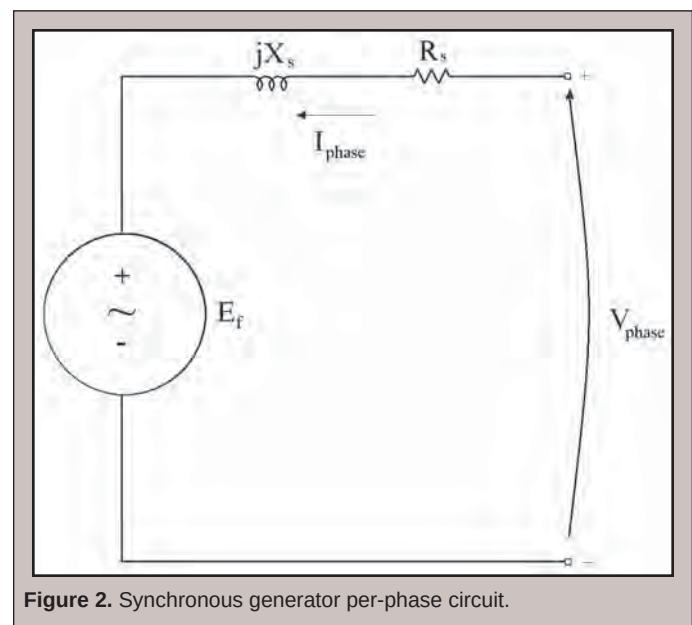


Figure 2. Synchronous generator per-phase circuit.

I_{phase} . Active power output was found by determining the losses in the circuit due to the resistive elements subtracted from the converted mechanical power. Reactive power was determined by a specified control mode. At this stage of development, a constant power factor control mode was used to determine the desired reactive power output of the generator. The power factor can be adjusted, within the limits of the generator's capabilities, to deliver or absorb reactive power as needed to meet the requirements of the control mode. The controller will be implemented at a later time using an external control module. Further development will also include constant potential and constant power modes, depending upon the application. These control modes can be considered analogous to generalized versions of common generator dispatch methods.

Induction Generator

The induction generator was also modeled using a balanced Y-configuration; however, unbalanced loading was not fully tested. The per-phase model is shown in Figure 3. Similar to the PMSG, V_{phase} is determined by the bus voltage, and I_{phase} is the desired output. The circuit is solved with the two-port matrix

$$\begin{bmatrix} V_{\text{phase}} \\ I_{\text{phase}} \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \times \begin{bmatrix} V_{\text{rotor}} \\ I_{\text{rotor}} \end{bmatrix}, \quad (7)$$

where the matrix elements are given by

$$\begin{aligned} a &= 1 + Z_{st} / Z_c & Z_c &= \frac{R_c \times jX_m}{R_c + jX_m} \\ b &= Z_r + Z_{st} + Z_{st} \cdot Z_r / Z_c & Z_r &= R_r + jX_r \\ c &= 1 / Z_c & Z_{st} &= R_{st} + jX_{st} \\ d &= 1 + Z_r / Z_c \end{aligned} \quad (8)$$

In this case, V_{rotor} is a representation of the voltage across the resistor which represents the power converted, not an actual potential. For development purposes, a constant power mode was used to generate the maximum amount of active power available at the terminals. Reactive power was then found for that level of active power. The circuit was once again solved iteratively, and per unit values were used.

RESULTS AND DISCUSSION

Four test turbines were designed: a generic 1.5 MW induction generator, a generic 1.5 MW synchronous generator, a 1.65 MW PMSG representation of a Vestas V82 turbine, and a 2.5 MW PMSG GE turbine. Vestas V82 wind turbines, which actually use DFIGs, were represented as PMSGs within the electrical portion of the model for testing purposes. GE and Vestas are the largest suppliers of wind turbines within the United States [14] and had the most data publicly available, making them the easiest to model at this stage. For this reason they were selected as two of the turbines to be included at this stage of development.

Initially, all of the models were tested as stand-alone modules. They were connected to a constant voltage infinite bus, where the constant voltage was held near the generator's rated terminal voltage. Both active and reactive power was then measured as a function of wind speed at standard air density and temperature. Where applicable, the outputs were compared to manufacturers' data (Figures 4–5). The generator and turbine specifications used are presented in Table 1. The Vestas V82 provided similar results to its manufacturer's data, except at high wind speeds (Figure 4a), where slight polynomial perturbations can be seen which were due to the low order polynomial interpolation of coefficient of performance data. Later implementations may employ other forms of interpolation from manufacturers' data to reduce the error at higher wind speeds. The GE 2.5 MW, on the other hand, provided similar results to its manufacturer's data at high wind speeds, but consistently provided lower power output at lesser wind speeds (Figure 4b). As discussed before, this is due to the use of the generalized, fixed pitch, coefficient of performance model to determine the percentage of mechanical power transferred. GE wind turbines use variable pitch blade systems, which increase the coefficient of performance at lower wind speeds and can provide a higher cut-off wind speed. This illustrates the advantages of using, variable pitch wind turbines with active control over fixed pitch turbines: more power can be consistently provided at lower wind speeds. Figure 5a illustrates the output of a fixed pitch, 1.5 MW PMSG wind turbine as a general model, while Figure 5b shows

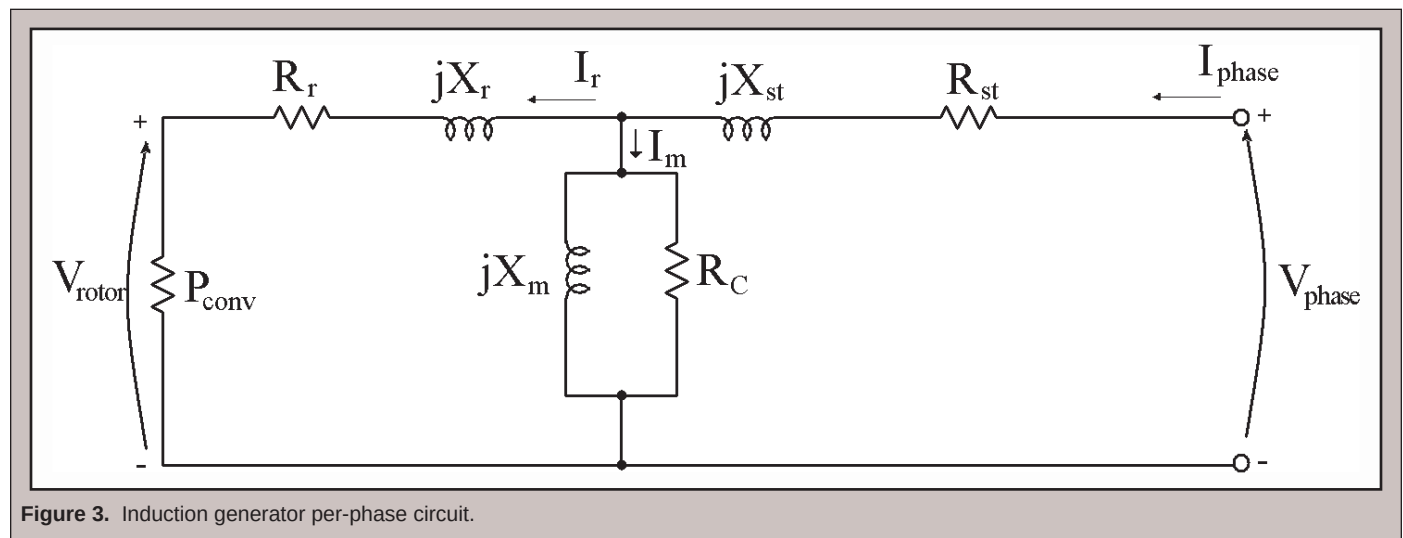


Figure 3. Induction generator per-phase circuit.

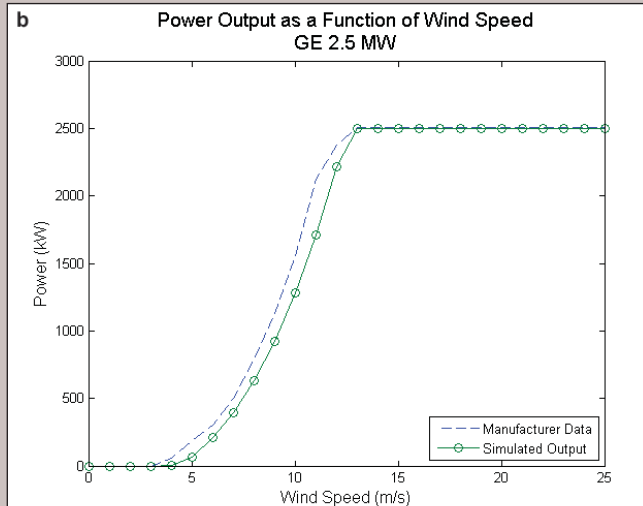
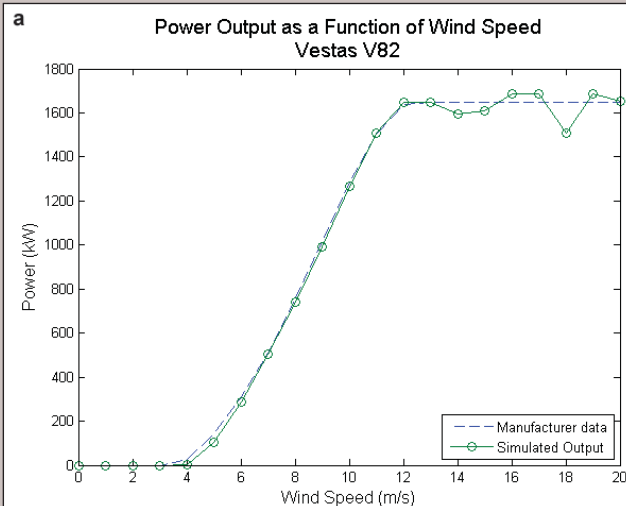


Figure 4. (a) Active power for Vestas V82 compared to manufacturer's data. (b) Active power for GE 2.5 MW compared to manufacturer's.

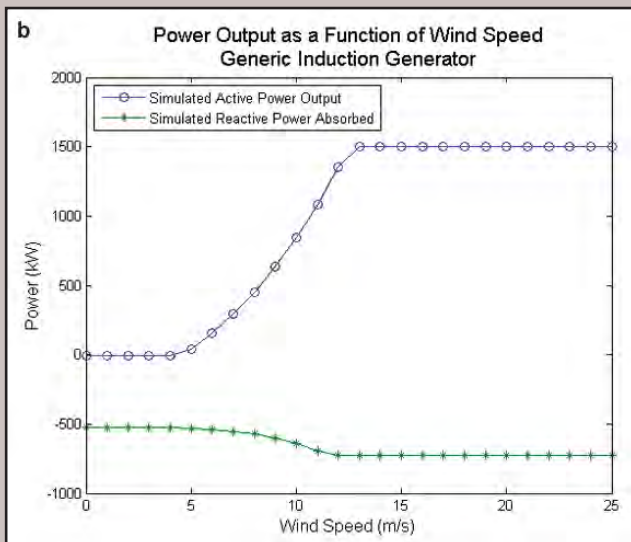
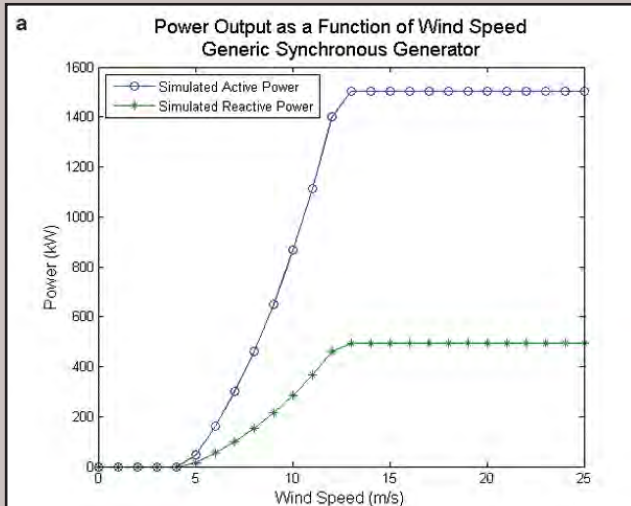


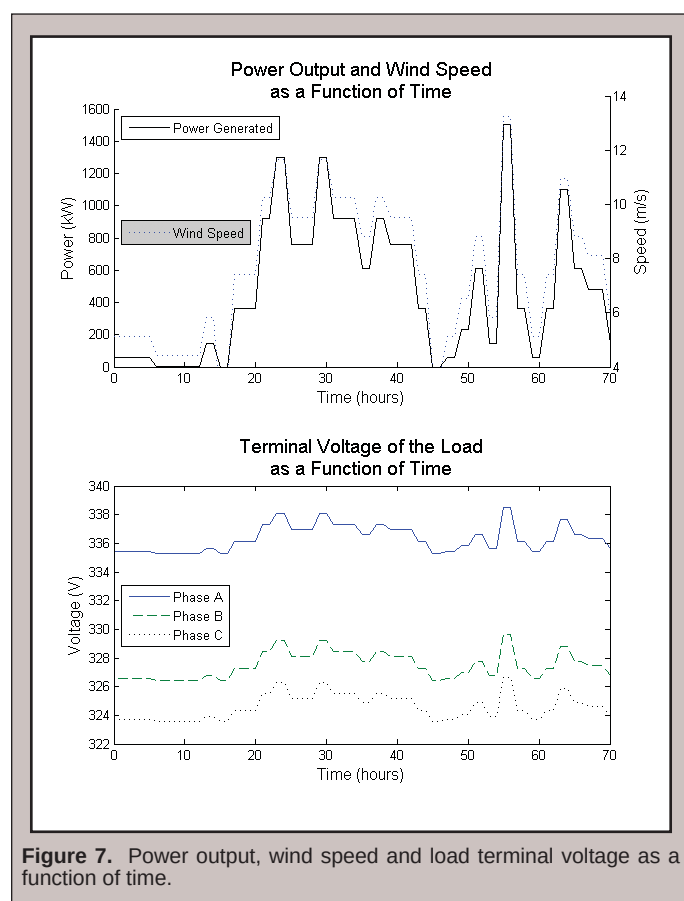
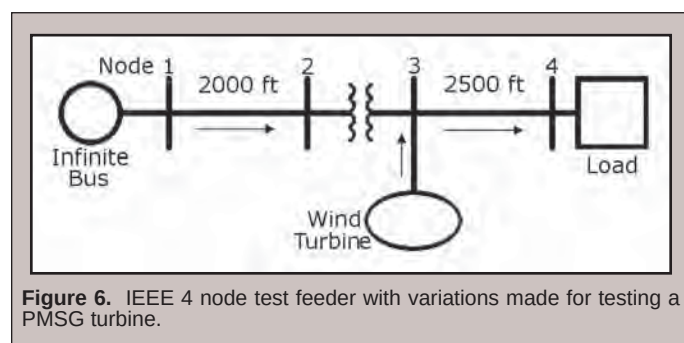
Figure 5. (a) Active and reactive power generated by the generic 1.5 MW PMSG. (b) Generic 1.5 MW induction generator, including active and reactive power.

	Vestas V82	GE 2.5	Synchronous	Induction
C. of Performance	Manufacturer	Justus	Justus	Justus
Generator Type	*Synchronous	Synchronous	Synchronous	Induction
Rated Power (MW)	1.65	2.5	1.5	1.5
Rated Voltage (V)	600	690	600	600
Rotor Diameter (m)	82	100	82.5	82.5
Cut In Wind Speed (m/s)	3.5	3.5	4	4
Rated Wind Speed (m/s)	13	12.5	12.5	12.5
Cut Out Wind Speed (m/s)	**20	25	25	25

Table 1. The generator and turbine specifications used for testing the models.
*In reality, Vestas uses a DFIG, but a PMSG representation was used.
**Ten minute cut out speed.

the active power output and reactive power absorption of a fixed pitch, 1.5 MW induction generator wind turbine. Since both these turbines represent generalized models, there is no data to compare. The models can be adjusted to represent almost any size turbine and it is up to the user to redefine them as needed for specific applications. In Figure 5, the induction generator active power is similar to that of a synchronous generator. The PMSG provides reactive power at similar curves to the active power, since it is controlled at a constant power factor of 0.95. However, in the induction generator, reactive power is continuously absorbed, somewhat independent of the wind speed. For this reason, induction machines are no longer commonly used as generators without additional shunt capacitors; however, the results in Figure 5 are consistent with an induction generator configuration. Further development of the wind turbine model will include DFIGs, which do not always consume reactive power and can actually provide reactive power when needed. This is one of the primary reasons they are finding widespread acceptance within the industry.

The PMSGs were also tested on a variation of the IEEE 4 node step-down test feeder (Figure 6) with an unbalanced load. The wind turbine generator was attached to node three. The secondary voltage on the Y-Y-connected transformer was changed to the rated voltage of the generator, and the unbalanced, constant power load was reduced to a level stable for that voltage. The entire feeder was then run using wind and temperature data from Tulsa, OK at one hour time step increments. Figure 7 shows the magnitude of the voltage of the three phases at the load, measured at each time step, and the corresponding power and wind speed at each step. As the wind turbine supplies more power to the system, the strain on the load voltage decreases and the voltage increases accordingly. Phase C has the largest load, and correspondingly, has the lowest voltage returned of the three phases.



CONCLUSION

Generic and manufacturer-specific aerodynamic models were created to simulate the mechanical power extracted from wind data provided by TMY2 sources, with sufficient corrections for atmospheric conditions, hub height and mechanical losses. Preliminary designs were created for both synchronous and induction generators to extract electrical power. These prototype models were tested against publicly available manufacturers' data and against a variation of the IEEE 4 node test feeder.

The model in this project created a generalized, first-run prototype, but further work is needed to accurately model the wind turbines that are available. The goal was to create a template for future designers, which can be used to create highly accurate, time varying models of specific turbine designs. The main future tasks will include the creation of a DFIG model, as these generators become more widely used, and the creation of more accurate control and dispatch methods. Future work will also include the integration of further atmospheric and location specific data, to account for variability in air density, especially at different geographical locations. Finally, more accurate models should be created to represent coefficient of performance data. For cases where data is not available, a variable pitch approximation should be designed, which, although case-specific for individual turbines, will provide a better approximation than a fixed pitch model.

New tools, such as GridLAB-D, coupled with models for new and existing technologies, are needed as more advanced technologies are integrated into the electricity infrastructure. As new technologies are created, such as Grid-Friendly™ appliances or plug-in hybrid vehicles, the effect of their integration will need to be studied in more accurate, time-sensitive detail. An open-source, next generation, power simulation system, like GridLAB-D, allows for a wider user base, faster and easier creation of simulation modules, and can assist in the integration of new technological capabilities.

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HEAD INJURY ASSESSMENT IN JUVENILE CHINOOK USING THE ALPHA II-SPECTRIN BIOMARKER: EFFECTS OF PRESSURE CHANGES AND PASSAGE THROUGH A REMOVABLE SPILLWAY WEIR

CHRISTINE JONASON AND ANN MIRACLE

ABSTRACT

The cytoskeletal protein alpha II-spectrin has specific neurodegenerative mechanisms that allow the necrotic (injury-induced) and apoptotic (non-injury-induced) pathways of proteolysis to be differentiated in an immunoblot. Consequently, α II-spectrin breakdown products (SBDPs) are potential biomarkers for diagnosing traumatic brain injury (TBI). The purpose of the following investigation, consisting of two studies, was to evaluate the utility of the spectrin biomarker in diagnosing TBI in fish that travel through hydroelectric dams in the Columbia and Snake Rivers. The first study used hyperbaric pressure chambers to simulate the pressure changes that affect fish during passage through a Federal Columbia River Power System (FCRPS) Kaplan turbine. The second study tested the effect of a removable spillway weir (RSW) on the passage of juvenile chinook (*Oncorhynchus tshawytscha*). This study was conducted in tandem with a balloon-tag study by the U.S. Army Corps of Engineers. Brain samples from fish were collected and analyzed using an immunoblot for SBDPs, and imaging software was used to quantify the protein band density and determine the ratio of cleaved protein to total protein. The biomarker analyses found higher SBDP expression levels in fish that were exposed to lower pressure nadirs and fish that passed through the RSW at a deep orientation. In general, the incidence of injuries observed after treatment positively correlated with expression levels, suggesting that the biomarker method of analysis is comparable to traditional methods of injury assessment. It was also found that, for some treatments, the 110 kDa spectrin fragment (SBDP 110) correlated more strongly with necrotic head injury incidence and mortality rates than did the total cleaved protein or the 120 kDa fragment. These studies will be informative in future decisions regarding the design of turbines and fish passage structures in hydroelectric dams and will hopefully contribute to the development of faster and more accurate techniques for diagnosing TBI in fish.

INTRODUCTION

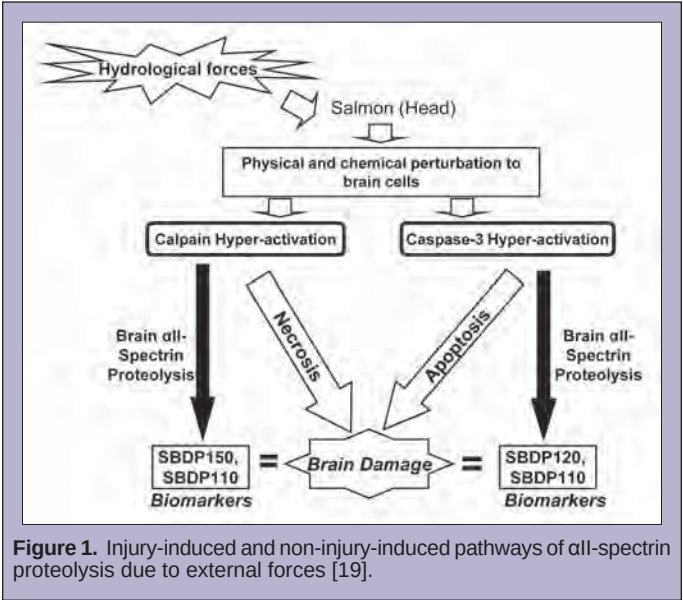
Salmonid species passing through hydroelectric dams on the Columbia and Snake Rivers in Washington face the possibility of injury and death from these structures. Fish that cannot find a surface outlet at the forebay of a dam resort to swimming under the turbines at greater depths than they are accustomed to [1], [2]. This can have potentially lethal effects on their physiology and behavior, causing changes in buoyancy, swim bladder rupture, disorientation, cold stress and abnormal swimming behavior [2]. Additionally, the rotating turbines can cause injury and mortality through sheer stress and collisions sustained during passage [3], [4], [5].

In an attempt to decrease the frequency of injury and mortality from dam passage, the U.S. Army Corps of Engineers (USACE) has constructed fish passages, such as adult fish ladders and juvenile

bypass systems, in eight of the 18 dams on the Columbia and Snake Rivers [6]–[8]. Evaluations of these structures usually involve observational studies in which the fish are tagged, released into the forebay and then recaptured and examined for injuries after swimming through the passage spillbay [4], [6], [9], [10]. These assessment methods are limited, though, in that they can diagnose only visible injuries, while fish may sustain subacute injuries, such as traumatic brain injuries, with no observable effects. Because of this limitation it is desirable to develop a molecular approach that goes beyond visible observations and produces a more quantitative assessment of the injuries that have occurred.

The solution to this problem may lie with a molecular marker of traumatic brain injury (TBI) known as the α II-spectrin biomarker, which has been studied extensively in mammals [11]–[17], but has

only recently been applied to research in fish [18], [19]. Alpha II-spectrin (α II-spectrin) is a subunit of the protein spectrin, which is found in axons and presynaptic terminals of the central nervous system [11]. The potential for using α II-spectrin as a biomarker for TBI emerges from the fact that proteolysis of the protein produces different-sized fragments when normal cell death occurs compared to when injury-induced cell death occurs. Proteolysis of α II-spectrin by means of a necrotic (injury-induced) pathway is mediated by calpains (calcium-dependent proteases with palpain activity) and is localized at the site of impact [11], [14]. In fish, this pathway produces 150 and 110 kDa protein fragments [18] (Figure 1). The apoptotic (non-injury-induced) pathway of cell death is mediated by calpains as well as by caspase-3, a cysteine protease. Apoptosis occurs in areas surrounding the impact site and results in 150, 120 and 110 kDa fragments [18]. These protein fragments, known as spectrin breakdown products (SBDPs), can be distinguished on an immunoblot and analyzed for density to determine their relative abundance in the brain tissue [11]–[19].



Previous studies involving mammalian systems have found that SBDP levels correlate with different types and severities of head injuries [14]–[17]. Based on these studies and preliminary results from Pacific Northwest National Laboratory (PNNL) [18], it was proposed that TBIs sustained by fish could be quantified based on differential analysis of expression of the 110 and 120 kDa SBDPs in brain tissue. The purpose of both studies described in this paper was to evaluate the effectiveness of the α II-spectrin biomarker at diagnosing incidences of TBI in juvenile chinook salmon (*Oncorhynchus tshawytscha*) and to determine if the biomarker can be used to quantify the severity of head injuries sustained during dam passage.

The first study was designed to simulate the rapid decompression experienced by fish swimming through a Federal Columbia River Power System (FCRPS) Kaplan turbine. Hyperbaric pressure chambers were used to acclimate fish to a standard pressure, representative of normal river conditions, and then subject them to a rapid decompression down to a typical nadir pressure. It was expected that lower nadir pressures would result in a higher incidence

of injury and mortality in the fish. Observations during necropsies of the fish were compared to molecular analysis to evaluate the effectiveness of the biomarker at detecting and quantifying these injuries.

The second study was conducted to evaluate the effects of a removable spillway weir (RSW) at Lower Monumental Dam on the Snake River. The RSW is considered more efficient than a traditional spillway in reducing migration delays [1]. The goal of this study was to quantify the SBDP expression levels among two treatment groups involving the RSW and one control group, in order to ultimately determine if TBI incidence was higher in fish that passed through the RSW. Additionally, visible signs of injury in the test fish were recorded, and the rate of observable passage-related injuries was compared to the molecular analysis order to assess the accuracy of the biomarker.

MATERIALS AND METHODS

Treatments and Tissue Collection, Pressure Study

The pressure study was conducted at PNNL from January 4 to February 4, 2008. Test fish ranged from 120 to 140 mm in length and came from a single cohort of hatchery-raised fish. The test fish were randomly assigned to seven treatment groups. Each group was placed in a hyperbaric pressure chamber and acclimated to a standard pressure of 21.2 psi in 123–125% total dissolved gas (TDG) for at least 16 hours. Control groups were acclimated along with treatment groups. These test conditions simulated passage at 15 feet below the surface of the water, with TDG exceeding 100% to simulate the turbulent, hyperoxygenated conditions of water moving through a turbine. After acclimation, a pressure spike was applied throughout all of the chambers except for those with control fish. The pressure started at 58 psi and decreased to a nadir between 2.1 and 14.31 psi, according to the designated treatment (Table 1). After testing, the fish were euthanized using 250 mg of

Test	Acclimation depth (ft)	Nadir (psi)	Total Dissolved Gas (%)	Class
997	15	2.1	124.5	extreme
989	15	2.59	124.76	extreme
978	15	3.32	125.22	extreme
1000	15	3.66	123.92	extreme
1005	15	12.21	124.25	intermediate
994	15	12.36	124.18	intermediate
1015	15	12.36	123.74	intermediate
981	15	12.75	123.61	intermediate
979	15	14.31	125.42	intermediate
995	15	33.13	124.47	intermediate
980	15	-999	123.75	control
1036	15	-999	125.39	control
1037	15	-999	124.98	control
1039	15	-999	125.4	control
1043	15	-999	123.38	control

Table 1. Pressure study tests, organized by classification. Acclimation pressure for all groups was 21.2 psi (15 ft).

MS-222 (tricaine methanesulfonate)/L of river water and necropsied. Afterwards each fish was decapitated and the brain was surgically extracted. Brain samples were transferred to cryotubes, flash-frozen in liquid nitrogen and stored at -80 °C.

Lower Monumental Dam Study

The USACE contracted with Normandeau Associates, Inc. (Normandeau) to conduct a balloon-tag study involving a new removable spillway weir (RSW) at Lower Monumental Dam (Kahlotus, Washington) during March 24–31, 2008. Juvenile hatchery chinook were obtained from Kooskia National Hatchery (mean fork length x 114 mm). They were tagged according to Normandeau's balloon-tag method [21] and sent through the RSW in groups of ten to fifteen at either "deep" or "mid" intake levels. After being captured downstream of the dam, the fish were held in tanks for 48 hours and then were briefly anaesthetized with clove oil and examined by Normandeau personnel for signs of injury. Control fish were tagged and released at the tailrace of the juvenile bypass system, captured downstream and then handled in the same manner. After observations were complete, a subset of these fish (30 per passage type) was euthanized and brain samples were extracted using the same procedure described for the pressure study.

Assessment of Head Trauma

Each fish in the pressure study was examined for swim bladder rupture and signs of embolism, hemorrhaging and hematoma in the gills, eyes and fins during necropsy. Injuries that were considered signs of head trauma included hemorrhaging and embolism in the eyes and exthalmia (eye popping). Head injuries were documented and later correlated with expression data obtained from the biomarker analysis. For the Lower Monumental study, the percent of fish sustaining passage-related maladies from each treatment was calculated from field data provided by Normandeau.

Protein Homogenization

Brain samples were homogenized using a MiniBeadBeater-8 and 1.0-mm Zirconia/Silica beads (BioSpec Products, Inc.). A 1X Triton protein extraction buffer (20 mM tris, pHx7.4, 150 mM NaCl, 5 mM EDTA, 5 mM EGTA, 1% TritonX-100) with protease inhibitors and 1.0 mM DTT was added to the sample before homogenization. The lysates were incubated on ice for 90 minutes and then centrifuged at 14000 rpm for 30 minutes at 4 °C. The protein concentrations of the supernatants were determined using the direct current protein assay (Bio-Rad) and a Genesys 10 UV scanning spectrophotometer (Thermo Scientific). After determining the protein concentrations, 20-µg aliquots of each sample were made and stored at -80 °C.

Immunoblot Technique

All samples were boiled for five minutes with loading buffer containing sodium dodecyl sulfate (SDS). Samples were loaded on polyacrylamide gels (4–15% Tris HCl, Criterion) and gel electrophoresis was conducted in a 10% Tris-glycine-SDS buffer (Sigma) at 125 V for two hours. After separation, the proteins were transferred onto a 0.45-µm polyvinylidene fluoride (PVDF) membrane (Pall Corporation) at 20 V for two hours using a blotter assembly (Criterion). The membrane was then blocked in 5% milk in Tris-buffered saline containing 0.05% Tween 20 (TBST, Sigma-Aldrich) for one hour and incubated for one hour with a mouse

polyclonal antibody for α II-spectrin (Banyan Biomarkers). Next the membrane was washed in TBST three times for five minutes each time and probed with a biotinylated secondary antibody (Banyan Biomarkers) for one hour. After completing the TBST washing procedure again, protein bands were detected by incubating the membrane with 5 mL of BCIP-NBT reagent (Banyan Biomarkers) for one to two minutes. The membranes were washed in deionized water and air-dried.

Protein Band Visualization

A digital picture of each gel was taken, and densitometric analysis of the bands was conducted using ImageJ software (version 1.6, National Institutes of Health), which quantifies the bands based on their relative intensities [13]. Densitometry values were recorded for the 280 kDa band (the intact protein) and the 120 and 110 kDa bands (the breakdown products). A final densitometric ratio was figured by determining the ratio of breakdown products (SBDP 120+SBDP 110) to total protein (intact 280 kDa+SBDP 120+SBDP 110). Additionally, the expression of each individual breakdown product was calculated by dividing each SBDP expression level by the sum of intact protein and that SBDP. For example, density values for the SBDP 110 band were divided by density values for intact 280 kDa+SBDP 110. Densitometry measurements were taken twice and averaged for each fish.

Statistical Analyses

After densitometric values for each sample were configured, a *t*-test (two-tailed, $\alpha \times 0.05$) was used to detect statistically significant variations in SBDP levels. The correlation of SBDP levels to observed injuries was calculated using a regression analysis in SigmaPlot 10.0 (Systat).

RESULTS

Pressure Study Results

Out of 161 fish that were exposed to the pressure treatments, 115 brain samples were assayed for the α II-spectrin biomarker. Figure 2 describes the range of densitometric values obtained from the biomarker analyses. Overall, the fish exposed to pressure treatments showed a higher level of expression of SBDP 110 and SBDP 120+SBDP 110 versus the control fish. The individual 110 and 120 kDa bands were able to distinguish between treatment groups with significant results for some, but not all, of the tests (Table 2). The level of observed head injuries was highest in fish that were exposed to lower pressure nadirs (the "extreme" treatments), and this trend correlates with the higher SBDP expression levels that were detected in the molecular analysis.

Lower Monumental Study Results

A total of 108 brain samples were collected from the Lower Monumental site: 90 mid-release, deep-release and control fish at 48 hours post-release on March 28, 2008, and 18 deep-release fish at 48 hours post-release on April 1, 2008 (Table 3). Figures 3 and 4 describe the range of densitometric values obtained from the biomarker analyses. There were two separate sampling days for fish from the deep treatments, indicated as deep day 1 and deep day 2. Statistical tests, as described above, compared the 120+110 densitometric values (i.e., the ratio of cleaved protein to total protein) and revealed significant differences between the control treatments

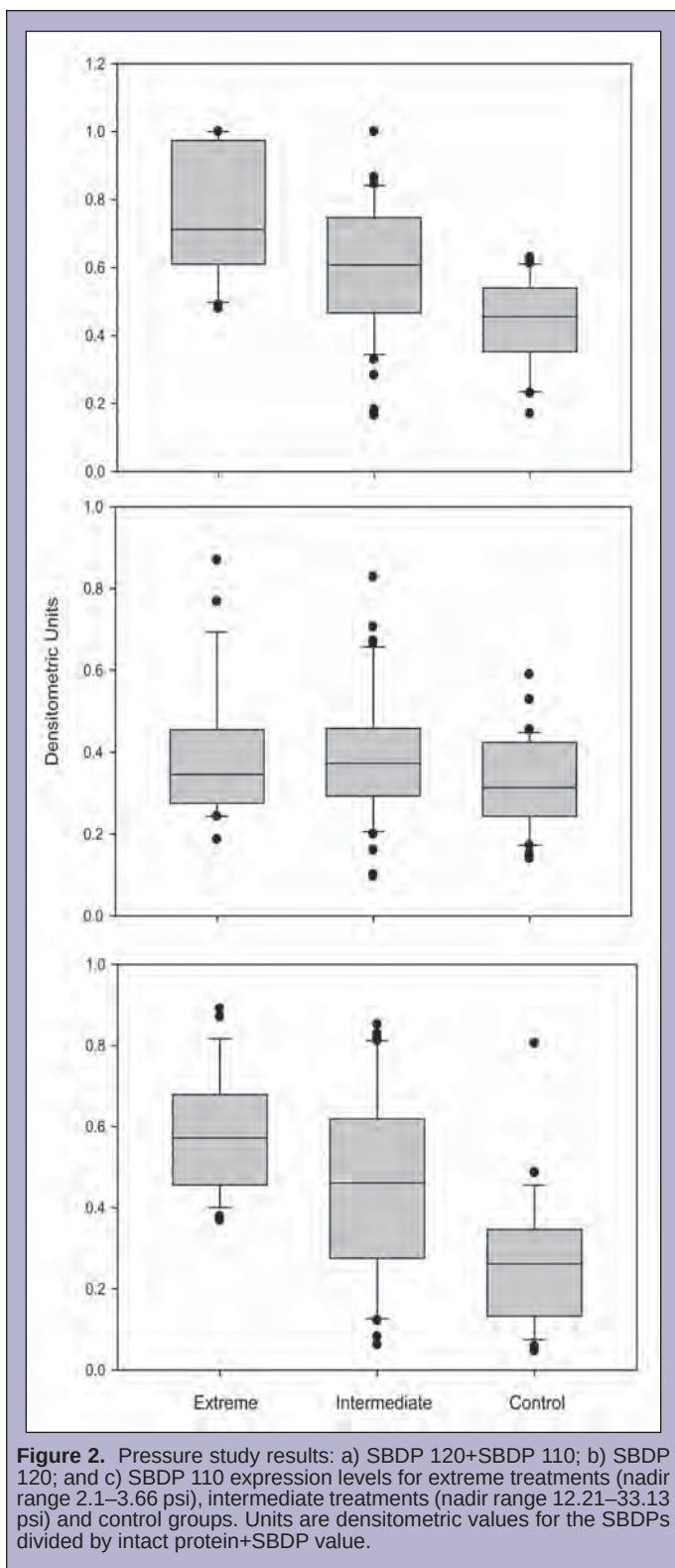


Figure 2. Pressure study results: a) SBDP 120+SBDP 110; b) SBDP 120; and c) SBDP 110 expression levels for extreme treatments (nadir range 2.1–3.66 psi), intermediate treatments (nadir range 12.21–33.13 psi) and control groups. Units are densitometric values for the SBDPs divided by intact protein+SBDP value.

and deep treatments (Table 4). The SBDP 110 densitometric ratios were significantly different between the control and mid groups, control and deep (separately and combined) and mid and deep (day 2 and both days combined) (Figure 4). Finally, the SBDP 120 densitometric values were significantly different between control and mid groups, control and deep day 2 and mid and deep (separately and combined) (Figure 4).

The rate of observed injury in the test fish positively correlated with expression levels of the SBDP 120+SBDP 110 biomarkers (i.e., the relative amount of cleaved protein compared to total protein). However, this correlation was not significant ($r^2 \times 0.78$, Figure 5).

DISCUSSION AND CONCLUSION

These studies evaluated the effectiveness of the α II-spectrin biomarker at quantifying the severity of head injuries sustained during two dam passage scenarios. The ratio of cleaved total protein (SBDP 120+SBDP 110) to intact protein (280 kDa) is indicative of α II-spectrin proteolysis as the result of either the apoptotic or necrotic pathway. Based on past work [18], [19], it is known that, in fish, the SBDP 120 fragment results from apoptotic pathway of cell death, while the SBDP 110 fragment results from both pathways.

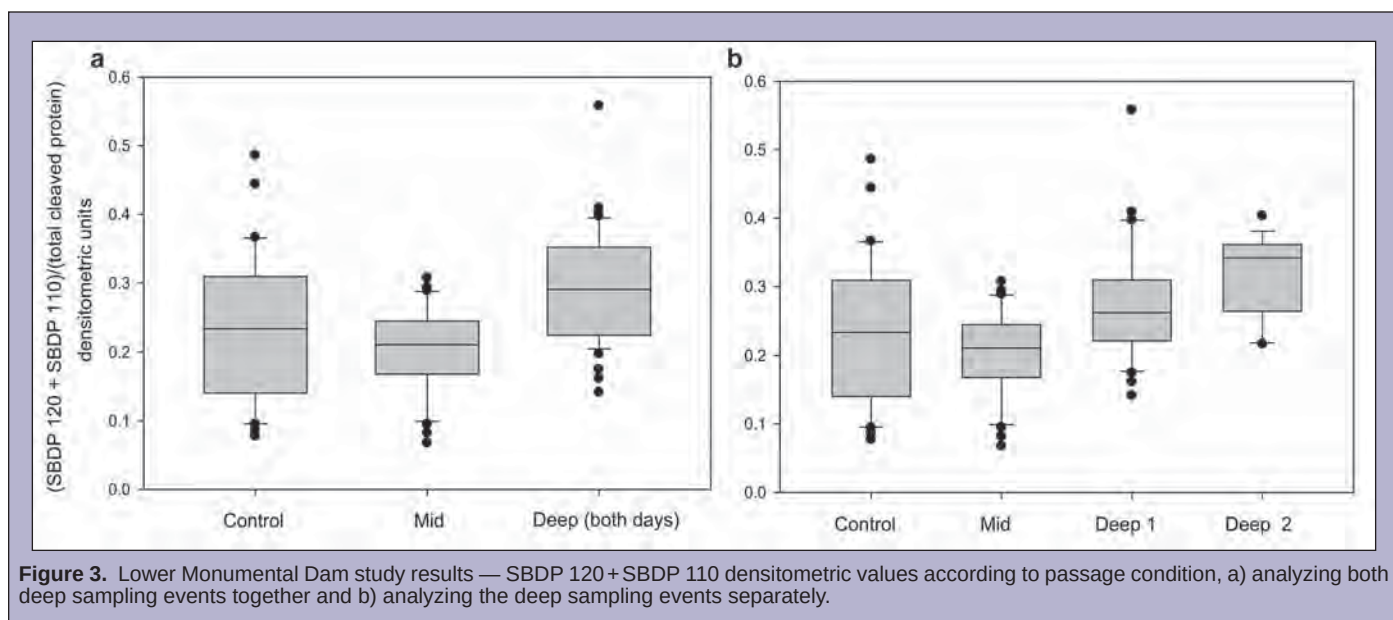
For both studies, the trends in SBDP expression levels accurately reflect the incidence of injuries observed in the fish after treatment. Additionally, in both studies at least one of the biomarker metrics (SBDP 110, SBDP 120, or total cleaved protein) was able to distinguish extreme treatments (low pressure nadirs or “deep” RSW level) from intermediate and control treatments, although not all results were significant. The results support a concept that emerged from research at McNary Dam [18], [19], that the α II-spectrin biomarker method is comparable to observational methods of injury assessment used for dam passage evaluations.

While biomarker expression from Lower Monumental passage treatments is positively correlated with observed injuries (Figure 5), the correlation is not as strong ($r^2 \times 0.78$) as it was in a 2007 study conducted at McNary Dam ($r^2 \times 0.91$) [18], [19]. Several factors may have contributed to this discrepancy. First, the biomarker detected a much higher incidence of subacute injury in the control fish from Lower Monumental than from the study at McNary. Whether this is due to differences in the passage type or to an actual increase in subacute injuries is unknown. The fish used for the Lower Monumental study were obtained from Kooskia National Fish Hatchery, had a mean length of 114 mm, and were generally in poor condition. Comparatively, the fish from McNary were from Little White Salmon hatchery, had a mean length of 140 mm, and were in relatively good condition [18], [19]. Either of these differences could have been a factor in the higher incidence of injuries. In any event, the higher levels of SBDP expression in control fish from Lower Monumental demonstrate that these fish were generally in poor health compared to the fish in the McNary study.

A second factor to consider when interpreting the Lower Monumental data is that the observed incidence of injury was very low for the day of the first deep release (deep day 1). Injury and malady data provided by Normandeau indicate a 5.5% injury in test fish from deep day 1, compared to a 17% injury in test fish from deep day 2 (Figure 5). When the second deep release date is considered separately, there is a marked increase in expression levels detected by the molecular assay which corresponds to the observed increase in injuries. Therefore, the incidence of injuries observed for deep day 1 correlate with the levels of SBDP expression on that day. For future studies it would be beneficial to sample fish from multiple release dates to ensure that a variety of passage-related injuries and maladies will be included in the analysis. Additionally, more consideration should be given to maintaining uninjured control fish to ensure an

SBDP 110	Extreme			Intermediate						Control						
	989	978	1000	1005	994	1015	981	979	995	980	1036	1037	1039	1043		
Extreme	997	0.0135	0.0215	0.0371	0.1224	0.0222	0.0054	0.8866	0.2657	0.0401	0.5693	3.59E-05	0.0011	0.0037	0.0012	
	989		0.4768	0.6937	0.0015	0.8549	9.54E-05	0.0595	0.7389	0.7898	0.1628	2.40E-06	3.14E-05	6.94E-05	5.23E-05	
	978			0.3193	0.0020	0.6004	1.88E-04	0.0389	0.4243	0.6921	0.0930	1.58E-05	1.25E-04	1.94E-04	2.54E-04	
	1000				0.0037	0.5933	2.09E-04	0.1057	0.9340	0.5640	0.2756	6.10E-06	8.48E-05	1.74E-04	1.66E-04	
Intermediate	1005					0.0021	0.0731	0.3539	0.0474	0.0039	0.1069	0.0036	0.0989	0.1322	0.3732	
	994						1.53E-04	0.0592	0.6609	0.9219	0.1529	6.73E-06	7.30E-05	1.35E-04	1.42E-04	
	1015							0.0335	2.99E-04	5.17E-04	0.0079	0.2042	0.6019	0.3872	0.1870	
	981								0.2632	0.0694	0.5803	0.0039	0.0396	0.0507	0.1079	
	979									0.6259	0.4885	8.65E-04	0.0058	0.0072	0.0137	
Control	980															
	1036											6.38E-04	0.0071	0.0103	0.0189	
	1037												0.0550	0.0733	0.0024	
	1039													0.9621	0.2159	
SBDP 120	Extreme			Intermediate						Control						
	989	978	1000	1005	994	1015	981	979	995	980	1036	1037	1039	1043		
Extreme	997	0.2955	0.0707	0.0604	0.1113	0.0806	0.8071	0.2274	0.0597	0.1066	0.3458	0.2374	0.1542	0.5453	0.0548	
	989		0.0703	0.1313	0.1986	0.1033	0.3539	0.6903	0.1542	0.1897	0.9692	0.0213	0.4134	0.9510	0.2097	
	978			0.2843	0.3193	0.6236	0.0413	0.1238	0.2594	0.3254	0.0989	0.0128	0.1488	0.1118	0.1599	
	1000				0.9694	0.5144	0.0786	0.2737	0.8254	0.9516	0.1813	0.0048	0.4796	0.3184	0.5403	
Intermediate	1005					0.5652	0.1025	0.3450	0.8238	0.9841	0.2519	0.0139	0.5206	0.3510	0.5847	
	994						0.0583	0.1852	0.4373	0.5761	0.1405	0.0120	0.2554	0.1838	0.2782	
	1015							0.2971	0.1096	0.1461	0.3893	0.6603	0.2675	0.2833	0.1560	
	981								0.3330	0.3329	0.7512	0.0212	0.6738	0.8665	0.4612	
	979									0.8060	0.2143	0.0045	0.6060	0.4077	0.6873	
Control	980															
	1036												0.0371	0.4823	0.9726	0.2824
	1037													0.0140	0.1480	0.0028
	1039														0.6355	0.8362
	</															

Table 2. P-values from t-tests comparing pressure study results (two-tailed, $\alpha=0.05$, assuming equal variance). Bold values indicate significant differences in SBDP 110 or SBDP 120 expression levels between treatment groups. Extreme and intermediate treatments are in order of increasing pressure nadir.



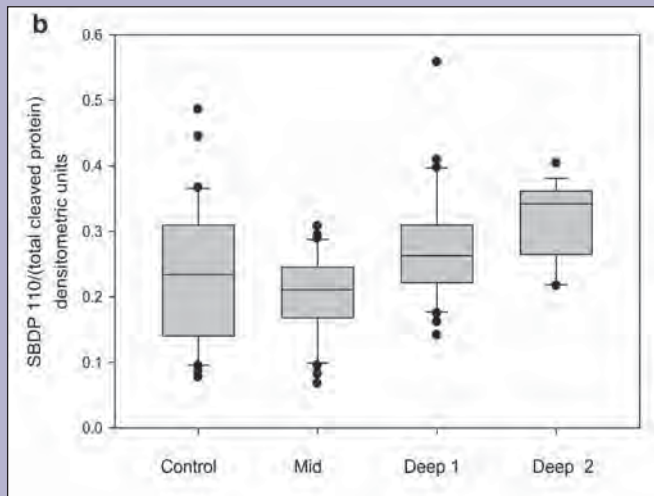
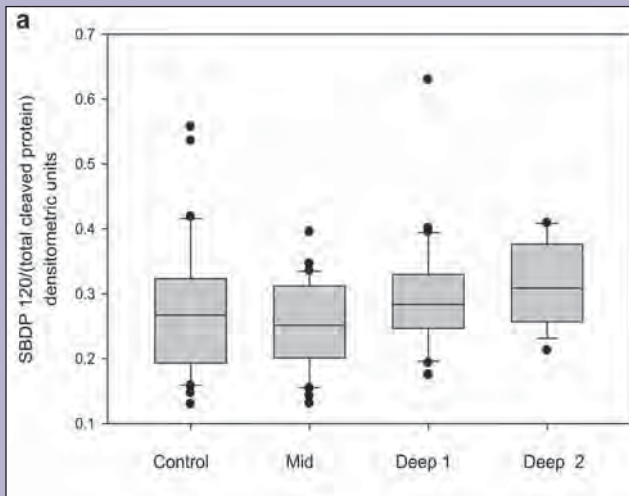


Figure 4. a) SBDP 120 and b) SBDP 110 densitometric values for treatment groups from the Lower Monumental Dam study at 48 hr post-release. SBDP 120 expression is indicative of the apoptotic pathway, while SBDP 110 indicates injury-induced (necrotic) cell death.

Route	Treatment	RSW discharge (cfs)	No. of fish collected at 48-hrs
RSW	Mid	8.7	30
RSW	Deep	8.7	48
Juvenile bypass pipe	Control	8.7	30

Table 3. Lower Monumental Dam study treatments.

SBDP120+110	Mid	Deep day 1	Deep day 2	Deep (both days)
Control	0.38	0.12	0.01	0.02
Mid		3.25E-03	2.15E-05	5.97E-05

SBDP 110	Mid	Deep day 1	Deep day 2	Deep (both days)
Control	0.21	0.08	4.10E-03	0.01
Mid		0.69	3.07E-03	1.20E-06

SBDP 120	Mid	Deep day 1	Deep day 2	Deep (both days)
Control	0.36	0.38	1.46E-01	0.17
Mid		0.04	2.03E-03	5.42E-03

Table 4. P-values from t-tests comparing densitometric values across treatment groups in the Lower Monumental Dam study (two-tailed, $\alpha \times 0.05$, assuming equal variance).

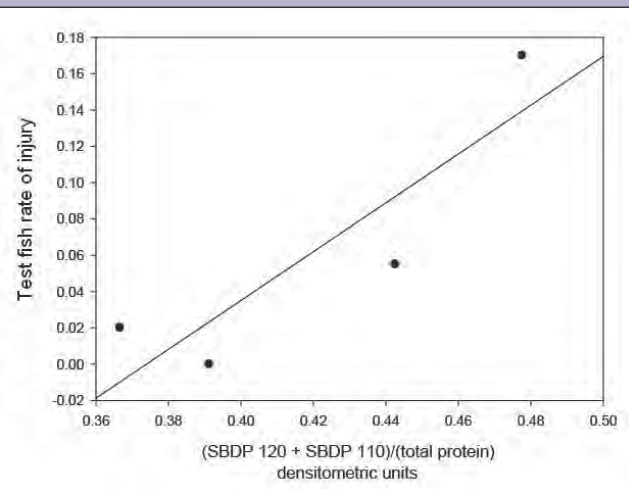


Figure 5. Correlation of protein densitometry (SBDP 120+SBDP 110) to observed incidence of injury across all treatment groups in the Lower Monumental Dam study ($R^2 \times 0.78$, $P \times 0.05$).

accurate background expression of biomarker levels for comparison to the treatments.

One development from these studies that was not previously observed is the utility of the 110 kDa breakdown product (SBDP 110), which in some treatments correlated more strongly with necrotic head injury incidence than the total cleaved protein or SBDP 120 alone. Results of the pressure study (Figure 2) demonstrate that total cleaved protein (SBDP 120+SBDP110) is higher in extreme treatments. However, it is clear from the plots of the individual biomarkers that this trend is driven almost completely by an increase in SBDP 110 expression rather than an increase in both SBDP 110 and SBDP 120. Furthermore, more of the extreme

and intermediate pressure study treatments had significantly higher expression levels compared to control treatments when the SBDP 110 metric was used (Table 2). Also, in the Lower Monumental study, biomarker expression levels from the “deep” RSW treatment are higher when the SBDP 110 metric is used (Figure 5).

Since the 110 kDa fragment is produced from the calpain-mediated necrotic pathway, this result is perhaps not surprising. Wang [22] found that calpain-mediated pathways are overactivated as a result of both necrotic and apoptotic pathways, so a higher expression of calpain-cleaved fragments would be expected after injury. Also, Pike, et al. [23] demonstrated that traumatic brain injury can increase calpain activity without increasing caspase activity, and according to Warren [16], the site of the injury may also contribute to the level of expression of certain SBDPs. From the current studies, there is no way of knowing if there is a threshold severity of injury that induces SBDP 110 expression in chinook, or if expression is dependent

on the type of injury, but these research questions would be worth exploring in future studies involving the α II-spectrin biomarker in fish.

These studies are some of the first to apply the use of a molecular biomarker to issues in wildlife management. Fish mitigation on the Columbia and Snake Rivers has been a goal of the USACE since construction of the dams began in the 1930s [6], and there are undeniable ecological and economic benefits to maintaining the populations of salmonid species in these waterways. Previous tests of an RSW at Lower Granite Dam showed a 98% survival rate in fish that used the RSW [1], and results from the study described here suggest that operating the RSW at a mid-level orientation will result in fewer incidences of head trauma and overall injury to juvenile fish. In terms of turbine design, past research [2], [3], [20] has demonstrated that fish that pass through a turbine on the suction side of the blade experience the lowest possible pressure nadirs from this trajectory. The observational and molecular results from the pressure study both demonstrate that low pressure profiles cause more internal injuries (swim bladder rupture, embolisms and hemorrhaging) and head trauma in fish. More information is needed about the distribution of fish entering turbines and the probability of exposure to a low pressure nadir and subsequent barotrauma before definitive guidelines can be developed [20], but results from this study imply that it would be best to design turbines that maintain high pressure profiles, or to increase altogether the use of fish screens, spillbays and bypass systems that divert fish from turbines.

There is great potential for development of the α II-spectrin biomarker as a method for assessing head injury in fish. The biomarker assay holds an advantage over traditional assessment methods because it can detect sublethal injuries and is a more cost-effective approach than using live fish for injury analysis. The studies described here essentially analyzed only short-term head injury impacts, but further research into this method may allow a threshold level of biomarker expression to be established, from which the probability of long-term survival for migrating fish populations could be estimated. Prospective research will also focus on developing rapid and non-lethal techniques for diagnosing TBI in fish by using the biomarker assay on blood samples rather than brain tissue samples. Finally, the observational studies and biomarker analyses from these studies have clearly demonstrated that low pressure nadirs and the “deep” RSW orientation result in higher incidences of injury in juvenile chinook salmon, and these results will be informative in future decisions regarding the design of turbines and fish passage structures in hydroelectric dams on the Columbia and Snake Rivers.

NOTE

All handling and processing of animals for this study was done in compliance with the Battelle Institutional Animal Care and Use Committee guidelines

ACKNOWLEDGMENTS

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A NEW METHOD FOR EXTRACTING SPIN-DEPENDENT NEUTRON STRUCTURE FUNCTIONS FROM NUCLEAR DATA

YONATAN F. KAHN AND WALLY MELNITCHOUK

ABSTRACT

High-energy electrons are currently the best probes of the internal structure of nucleons (protons and neutrons). By collecting data on electrons scattering off light nuclei, such as deuterium and helium, one can extract structure functions (SFs), which encode information about the quarks that make up the nucleon. Spin-dependent SFs, which depend on the relative polarization of the electron beam and the target nucleus, encode quark spins. Proton SFs can be measured directly from electron-proton scattering, but those of the neutron must be extracted from proton data and deuterium or helium-3 data because free neutron targets do not exist. At present, there is no reliable method for accurately determining spin-dependent neutron SFs in the low-momentum-transfer regime, where nucleon resonances are prominent and the functions are not smooth. The focus of this study was to develop a new method for extracting spin-dependent neutron SFs from nuclear data. An approximate convolution formula for nuclear SFs reduces the problem to an integral equation, for which a recursive solution method was designed. The method was then applied to recent data from proton and deuterium scattering experiments to perform a preliminary extraction of spin-dependent neutron SFs in the resonance region. The extraction method was found to reliably converge for arbitrary test functions, and the validity of the extraction from data was verified using a Bjorken integral, which relates integrals of SFs to a known quantity. This new information on neutron structure could be used to assess quark-hadron duality for the neutron, which requires detailed knowledge of SFs in all kinematic regimes.

INTRODUCTION

The study of nucleon structure functions (SFs) through inelastic electron scattering experiments has precipitated a series of remarkable insights into the nature of quarks and the strong force which governs their interactions. In particular, the phenomenon of quark-hadron duality has provided an opportunity to study the transition between the perturbative regime of quantum chromodynamics (QCD), which is probed in high-energy scattering experiments, and the non-perturbative regime, where quarks are confined and the strong force is realized as an exchange of mesons between hadrons. In 1970, Bloom and Gilman [1] noticed that proton SFs in the low-momentum-transfer (low- Q^2) regime, where the cross-section is dominated by nucleon resonances, averaged almost exactly to the SFs at very high Q^2 , where electrons were scattering off essentially free quarks. Since QCD at high Q^2 can be treated perturbatively, but

QCD at low Q^2 is highly non-perturbative, this observation provided an intimate link between the two regimes. Further investigation, fueled by increasingly accurate data, showed that [2] duality holds to some degree for spin-dependent as well as spin-independent proton SFs, through an extremely wide range of Q^2 , and in some cases for individual resonances over a limited range of x .

Duality is so far well-established for the proton but not as well for the neutron [2]. The lack of free neutron targets means that the analogous SFs for the neutron must be inferred from data on nuclear scattering. A method exists [3], [4] for extracting spin-averaged SFs, which are positive definite, but the method fails for spin-dependent SFs, which, as a difference of cross-sections, can have several zeros. In this paper, a new method is presented for extracting the spin-dependent neutron SFs g_1^n and g_2^n , both in the resonance and the deep inelastic scattering (DIS) region. A model of a nucleus, A , is

used where g_i^A are written as convolutions of spin-dependent nucleon momentum distributions, f_{ip} with g_j^p and g_j^n , where $i,j=1,2$. This reduces the problem to solving a system of integral equations, for which existing solution methods are reviewed and the new method is presented. The results of the method are illustrated on test functions and deuterium data from Thomas Jefferson National Laboratory (TJNAF) experiments, and it is shown that the results obtained are consistent with theoretical expectations. Concluding remarks are made on the application of this work to assessing quark-hadron duality for the neutron.

MATERIALS AND METHODS

Notation and Structure Function Formulas

While the experimental variables measured in inelastic electron-nucleus scattering are E' and θ (the outgoing electron energy and scattering angle respectively), the more theoretically useful quantities are Lorentz invariants. Figure 1 shows the lowest-order Feynman diagram that describes this process. l and l' are the incoming and outgoing electron 4-vectors, respectively, $q=l-l'$ is the 4-vector of the exchanged photon, p is the incoming nucleus A , and W is the sum of the 4-vectors of all outgoing particles except the electron. For relativistic electrons, $q^2 < 0$, so $Q^2 = -q^2$ is always positive. Another useful quantity is $\nu = (p \cdot q)/M_A$, where M_A is the mass of the nucleus; in the lab frame, ν is the energy transfer, $\nu = E - E'$. One can take ν and Q^2 to be the two independent variables describing the scattering process.

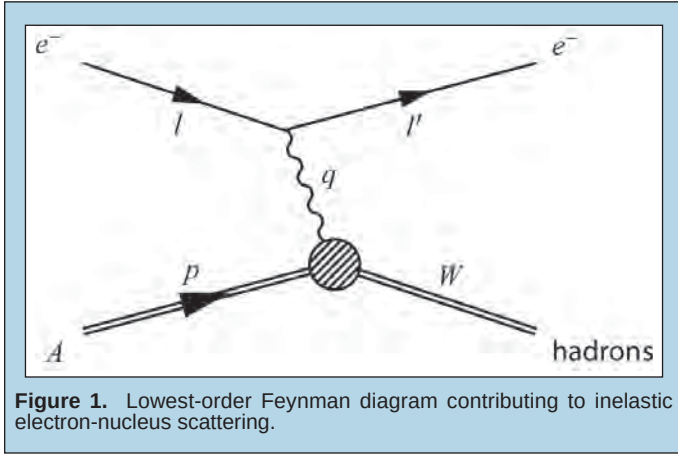


Figure 1. Lowest-order Feynman diagram contributing to inelastic electron-nucleus scattering.

In the impulse approximation of electron-nucleus scattering (Figure 2), the exchanged photon only interacts with one nucleon within the nucleus. Let k be the 4-momentum of the struck nucleon, and define $x_A = \frac{Q^2}{2p \cdot q} = \frac{Q^2}{2M_A \nu}$, $x_N = \frac{M_A}{M_N} \frac{Q^2}{2p \cdot q}$ and $y = \frac{M_A}{M_N} \frac{k \cdot q}{p \cdot q}$, where M_N is the mass of the nucleon. At very high Q^2 (the DIS region, hereafter referred to as simply DIS), the photon interacts with a single quark within the struck nucleon. Defining the z -axis as the direction of the incoming electron, it can be shown that as $Q^2 \rightarrow \infty$, and in a reference frame where $p_z \rightarrow \infty$, x_N/y is the fraction of the struck nucleon's z -momentum carried by the struck quark, and y is (up to a constant factor) the fraction of the nucleus' z -momentum carried by the struck nucleon. For kinematic reasons, $0 \leq x_A \leq 1$ and $0 \leq x_N, y \leq M_A/M_N$.

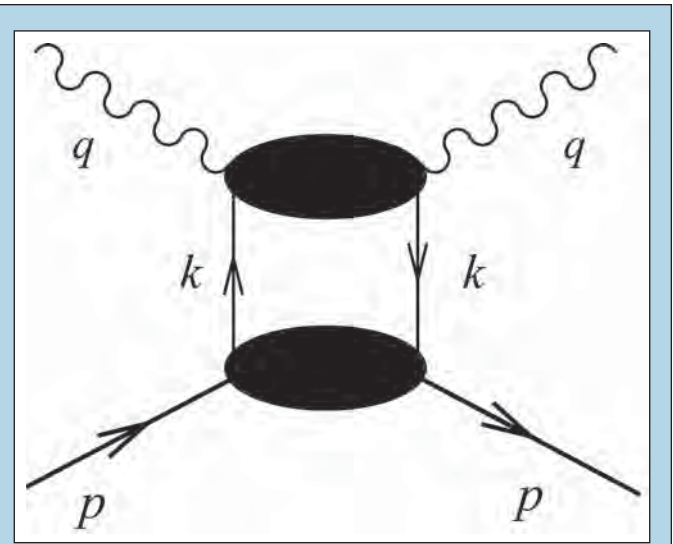


Figure 2. "Handbag" diagram of the impulse approximation for electron-nucleus scattering. This diagram represents the *squared* amplitude for the process; the left half corresponds to the blob in Figure 1, and squaring this amplitude gives the mirror image on the right-hand side.

The SFs mentioned in the introduction are related to the cross-sections for the inelastic scattering processes described above. The Feynman diagram in Figure 1 corresponds to a quantum-mechanical amplitude $\mathcal{M}$ for the scattering process to occur. The square of this amplitude can be factored as a product of tensors, $\mathcal{M}^2 = L_{\mu\nu} W^{\mu\nu}$, where $L_{\mu\nu}$ describes the electron vertex (the top of the diagram) and $W^{\mu\nu}$ describes the hadronic vertex (the bottom). $L_{\mu\nu}$ can be calculated directly from quantum electrodynamics and is well-understood, while $W^{\mu\nu}$ must be described empirically in terms of SFs because the underlying QCD processes cannot be calculated exactly. The most general Lorentz-covariant tensor satisfying the symmetries required by QCD can be written as

$$W^{\mu\nu} = W_1(\nu, Q^2) \left(\frac{q^\mu q^\nu}{q^2} - g^{\mu\nu} \right) + W_2(\nu, Q^2) \frac{1}{M^2} \left(p^\mu - \frac{p \cdot q}{q^2} q^\mu \right) \left(p^\nu - \frac{p \cdot q}{q^2} q^\nu \right) + i \epsilon^{\mu\nu\alpha\beta} \frac{q_\alpha p_\beta}{p \cdot q} \left(g_1(x, Q^2) s_\beta + g_2(x, Q^2) \left[s_\beta - \frac{s \cdot q}{p \cdot q} p_\beta \right] \right) \quad (1)$$

from which one can define the spin-averaged SFs $F_1(x, Q^2) := MW_1(\nu, Q^2)$ and $F_2(x, Q^2) := \nu W_2(\nu, Q^2)$, and the spin-dependent SFs $g_1(x, Q^2)$ and $g_2(x, Q^2)$. If either the electron beam or the target is unpolarized, only the symmetric part of $W^{\mu\nu}$ (the first line of equation (1)) contributes to the cross-section, so to access the g_p , one must measure a difference of polarized cross-sections:

$$\frac{d^2\sigma^{\uparrow\downarrow}}{d\Omega dE'} - \frac{d^2\sigma^{\uparrow\uparrow}}{d\Omega dE'} = \sigma_{Mott} \frac{4}{M\nu} \tan^2 \left(\frac{\theta}{2} \right) ([E + E' \cos \theta] g_1(x, Q^2) - 2Mxg_2(x, Q^2)). \quad (2)$$

In equation (2), the terms on the left hand side (LHS) are the cross-sections for scattering of electrons polarized antiparallel and parallel to the target, respectively, and σ_{Mott} is the cross-section for relativistic scattering off a point particle. The above formulas

are valid for both nucleon and nuclear targets, with $x = \frac{Q^2}{2p \cdot q}$, but for nuclear targets the SFs are usually expressed in terms of x_N , the *nucleon* variable, not x_A . Following this convention, for the remainder of this paper $x \equiv x_N$ is understood.

Convolution Formulas and Existing Extraction Methods

The framework of [5] is used to describe nuclear SFs in terms of nucleon SFs:

$$S_i^A(x, Q^2) = \sum_{j=1}^2 \int_x^{y_{\max}} f_{ij}^{p/d}(y, \gamma) S_j^p\left(\frac{x}{y}, Q^2\right) dy + \sum_{j=1}^2 \int_x^{y_{\max}} f_{ij}^{n/d}(y, \gamma) S_j^n\left(\frac{x}{y}, Q^2\right) dy \quad (3)$$

where A denotes any nucleus (for deuterium, the symbol d is used), the superscripts p and n denote the proton and the neutron, and $i, j = 1, 2$ index the SFs. $\gamma \equiv |\vec{q}|/q_0 = \sqrt{1 + 4 M_N^2 x^2 / Q^2}$ is a kinematical factor, and $y_{\max} = M_A / M_N$ is approximately the mass number of the nucleus. The lower limit of integration, $y_{\min} = x$, reflects the fact that the struck quark within the struck nucleon cannot have more momentum than the struck nucleon itself. S_i is a generic label for either the spin-averaged SFs: $x F_1 \equiv S_1$, $F_2 \equiv S_2$ or the spin-dependent SFs: $x g_1 \equiv S_1$, $x g_2 \equiv S_2$. In the following, for ease of notation we suppress the dependence of S_i on Q^2 , and note that equation (3) can be viewed as an equation in the single independent variable x for fixed values of Q^2 . The functions f_{ij} (referred to from now on as *smearing functions*) can be calculated from the wavefunction of the target nucleus, and are shown in Figure 3 for spin-dependent scattering off the deuteron. Note that the diagonal functions f_{11} and f_{22} are sharply peaked at $y = 1$. In a simple model where the nucleus is treated as a sum of free nucleons, these functions are Dirac delta

functions: $f_{11}(y) = f_{22}(y) = \delta(y-1)$. Also, the off-diagonal functions f_{12} and f_{21} are small in magnitude compared to the diagonal ones. Both of these observations are general features of the model and apply to any nucleus.

To extract the neutron SFs from proton and nuclear data at a given Q^2 , one convolutes (or *smears*) the proton SFs with the smearing functions and subtracts this contribution $\tilde{S}_1^p(x)$ (the first term on the right hand side (RHS) of equation (3)) from the nuclear SFs to obtain an effective smeared neutron SF $\tilde{S}_1^n(x) = S_1^d(x) - \tilde{S}_1^p(x)$. One then solves the system of equations

$$\tilde{S}_1^n(x) = \sum_{j=1}^2 \int_x^{y_{\max}} f_{1j}^{n/d}(y, \gamma) S_j^n\left(\frac{x}{y}\right) dy \quad (4)$$

for $S_j^n(x)$. Note that for a fixed Q^2 , γ is a function of x alone, so the smearing functions acquire an x -dependence. Equation (4) is a system of so-called Volterra integral equations of the first kind, which take the general form

$$g(x) = \int_x^a K(x, t) f(t) dt, \quad (5)$$

where $g(x)$ and $K(x, t)$ (the kernel) are known functions and f is unknown. The general theory of Volterra equations is quite extensive, see [6]. Most Volterra equations have no closed-form solution, but numerical solutions for first-kind equations are quite simple. Dividing the interval, $0 < y < y_{\max}$ into a grid of width h by $y_a = ah$, $a = 0, 1, \dots, N$, and using a quadrature method such as the trapezoidal rule or Simpson's rule, one can approximate the integral in equation (5) by a discrete sum

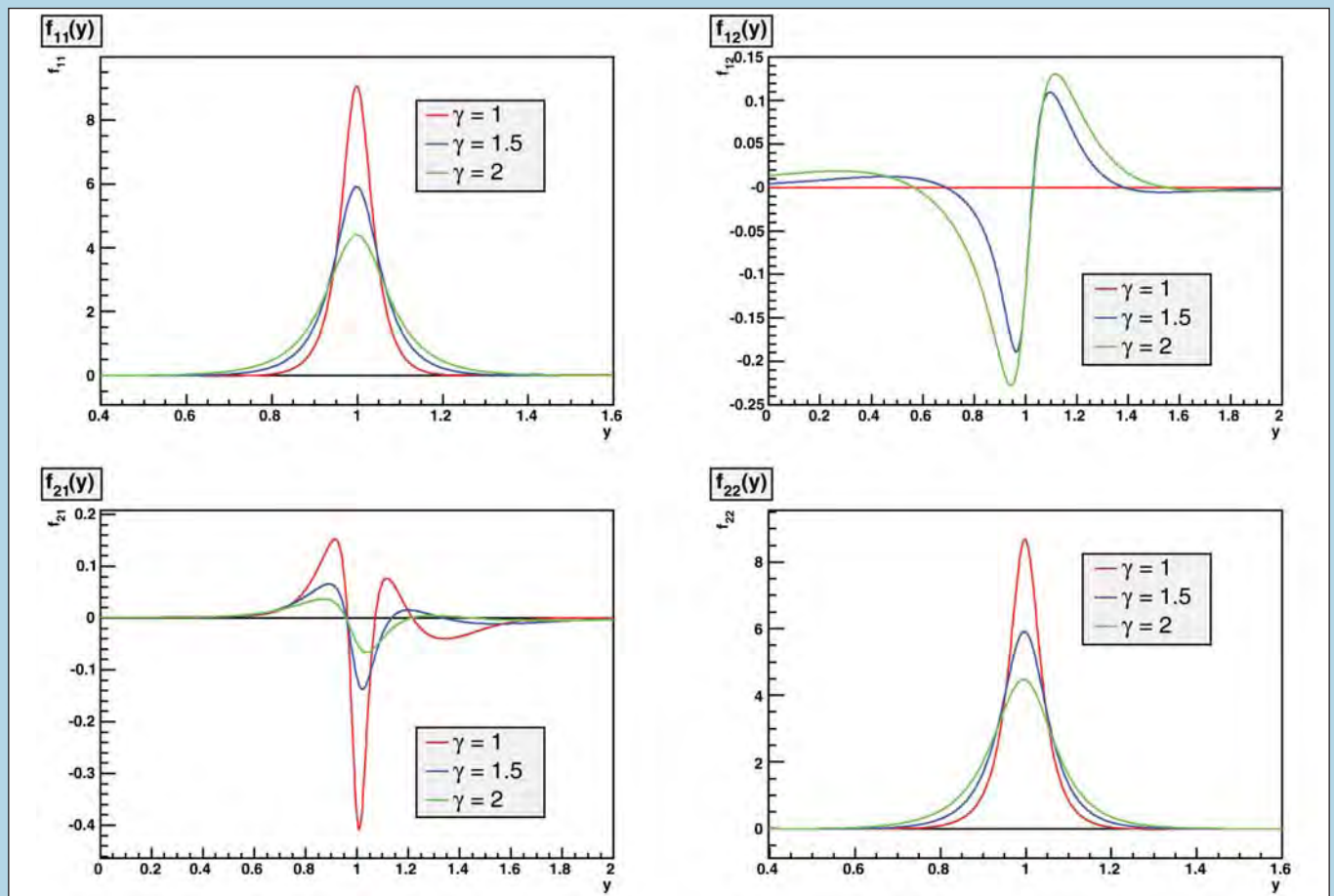


Figure 3. Spin-dependent deuteron smearing functions for various values of γ .

$$g_a = \sum_{b=a}^N K_{ab} f_b \quad (6)$$

thus reducing the numerical solution to a problem of matrix inversion: $\mathbf{f} = \mathbf{K}^{-1}\mathbf{g}$. In fact, because of the variable lower limit of integration, $y = x$, the matrix $\mathbf{K}$ is upper-triangular, and the inversion is almost trivial. This method has been tried by Ciofi degli Atti, et. al. [7] for a different smearing-function model. However, the method fails if $\mathbf{K}$ is singular.

Letting $t = x/y$, $v = x/y_{\max}$, equation (4) can be expressed in the form of equation (5):

$$\tilde{S}_i^n(y_{\max}, v) = \sum_{j=1}^2 \int_v^1 f_{ij}^{nA} \left(\frac{y_{\max} v}{t}, \gamma \right) \frac{y_{\max} v}{t^2} S_j^n(t) dt, \quad (7)$$

so the kernel is a sum of terms $K_{ij}(v, t) = \left(\frac{y_{\max} v}{t^2} \right) f_{ij} \left(\frac{y_{\max} v}{t}, \gamma \right)$. The diagonal $K_{ij}(v, v) \propto f(y_{\max})$ corresponds to the diagonal elements K_{bb} in the discretized equation (6). However, for any value of γ , $f(y_{\max})$ is extremely small for strong physical reasons: a single nucleon has a vanishing probability of carrying the entire momentum of the nucleus. Thus the matrix $\mathbf{K}$ has very small values along the diagonal and is very close to singular, so this solution method fails. A standard technique for Volterra equations with a kernel vanishing identically along the diagonal is to either integrate equation (7) by parts, or differentiate with respect to x ; the first approach gives an integral equation for the primitive of $S_j^n(x)$ with kernel $\frac{\partial}{\partial t} K(x, t)$,

while the second has kernel $\frac{\partial}{\partial x} K(x, t)$ and LHS $\frac{d}{dx} \tilde{S}_i^n(x)$. These manipulations are still problematic, because derivatives of the smearing functions are still very small at $y = y_{\max}$. Additionally, taking derivatives of functions that have been derived from fits to data introduces substantial errors. Furthermore, the solution depends on knowing $\tilde{S}_i^n(x)$ at *all* values of x , while in practice, only data up to $x = 1$ are available. These arguments show that a direct solution to equation (4) is impractical for the particular forms of smearing functions used in this model.

The most widely-used method for extracting spin-averaged SFs is known as the smearing-factor method [3], [4], referred to from now on as the *multiplicative method*. It is an iterative solution method based on the ansatz that the RHS of equation (4) can be written as a product of the neutron SF and an x -dependent “smearing factor” $Q(x)$:

$$\int_x^{y_{\max}} f_i^{nA}(y, \gamma) S_i^n \left(\frac{x}{y} \right) dy := Q(x) S_i^n(x). \quad (8)$$

There is no summation over $j = 1, 2$ in equation (8) since this method has only been applied for models where there are no off-diagonal smearing functions (call this the *single-unknown case*). From a first guess $S_i^{n(0)}(x)$, one obtains $Q^{(0)}(x)$ by smearing $S_i^{n(0)}(x)$ and dividing by $S_i^{n(0)}(x)$. Dividing $\tilde{S}_i^n(x)$ by $Q^{(0)}$ gives $S_i^{n(1)}(x)$, so the result after one iteration is

$$S_i^{n(1)}(x) = \tilde{S}_i^n(x) \frac{S_i^{n(0)}(x)}{\int_x^{y_{\max}} f_i^{nA}(y, \gamma) S_i^{n(0)} \left(\frac{x}{y} \right) dy}. \quad (9)$$

From the form of equation (9), it is clear this method is problematic if the smeared SF has zeros in the range of x of interest. The spin-averaged nuclear SFs are positive-definite for $0 < x < 1$, so this problem does not arise, and the multiplicative method converges

quite rapidly for essentially any reasonable choice of $S_i^{n(0)}(x)$. Even for spin-dependent SFs, which may have several zeros, the multiplicative method works fine *as long as the zeros of the smeared $S_i^{n(0)}(x)$ are very close to the zeros of $\tilde{S}_i^n(x)$* . Since the smearing functions are close to delta functions, this amounts to requiring that the zeros of the neutron SF be very close to the zeros of the nuclear SF. This may be the case in theory, but because of experimental errors it is certainly not the case in practice. An extraction method which avoids this problem is presented below.

Additive Extraction Method

Instead of assuming a multiplicative smearing factor, use the ansatz

$$\int_x^{y_{\max}} f_i^{nA}(y, \gamma) S_i^n \left(\frac{x}{y} \right) dy := \langle \sigma_i \rangle (S_i^n(x) + \delta(x)) \quad (10)$$

which defines an additive correction $\delta(x)$; here $\langle \sigma_i \rangle = \int_0^{y_{\max}} f_i^{nA}(y, \gamma) dy$. Starting from a first guess $S_i^{n(0)}(x)$, one obtains:

$$\delta^{(0)}(x) = \frac{1}{\langle \sigma_i \rangle} \int_x^{y_{\max}} f_i^{nA}(y, \gamma) S_i^{n(0)} \left(\frac{x}{y} \right) dy - S_i^{n(0)}(x); \quad (11)$$

$$S_i^{n(1)}(x) = \frac{1}{\langle \sigma_i \rangle} \tilde{S}_i^n(x) - \delta^{(0)}(x), \quad (12)$$

which gives, after one iteration

$$S_i^{n(1)}(x) = S_i^{n(0)}(x) + \frac{1}{\langle \sigma_i \rangle} \left(\tilde{S}_i^n(x) - \int_x^{y_{\max}} f_i^{nA}(y, \gamma) S_i^{n(0)} \left(\frac{x}{y} \right) dy \right). \quad (13)$$

Here, there is no danger of divergences due to zeros in the input, because the only division is by $\langle \sigma_i \rangle$, which is nonzero for all smearing functions $f(y)$. To solve the system of equations (4) (the *two-unknown case*), here written out explicitly as:

$$\tilde{S}_1^n(x) = \int_x^{y_{\max}} f_{11}^{nA}(y, \gamma) S_1^n \left(\frac{x}{y} \right) dy + \int_x^{y_{\max}} f_{12}^{nA}(y, \gamma) S_2^n \left(\frac{x}{y} \right) dy, \quad (14)$$

$$\tilde{S}_2^n(x) = \int_x^{y_{\max}} f_{21}^{nA}(y, \gamma) S_1^n \left(\frac{x}{y} \right) dy + \int_x^{y_{\max}} f_{22}^{nA}(y, \gamma) S_2^n \left(\frac{x}{y} \right) dy, \quad (15)$$

note that f_{11} is the most sharply peaked of the smearing functions, and hence will give the largest contribution to the RHS of equation (14). Assuming that the f_{12} contribution is zero, apply equation (13) to equation (14) (using $\langle \sigma_{11} \rangle$) to obtain $S_1^{n(1)}(x)$, which is plugged into equation (15). Subtracting this contribution from the LHS and applying equation (13) to equation (15) (using $\langle \sigma_{22} \rangle$) gives $S_2^{n(1)}(x)$. $S_2^{n(1)}(x)$ is then plugged into equation (14) and the recursive procedure is repeated.

The above single-unknown and two-unknown iterative solution methods were implemented in C++ using the spin-dependent deuteron smearing functions $f_{ij}^{n/d}(y, \gamma)$. The final C++ program took the smearing functions $f_{ij}^{n/d}$, SFs S_i^d and S_i^p , and a first guess $S_i^{n(0)}$ as input. The output was the extracted neutron SF S_i^n for a chosen number of iterations. The required integrals were computed using the trapezoidal rule with a grid spacing of $\Delta y = 0.002$ and the smearing functions were calculated with Mathematica from the formulas found in Kulagin and Melnitchouk [5] on a grid with spacing $\Delta y = 0.002$, for 14 discrete γ values. For both the test functions and parameterizations of real data, a grid spacing of $\Delta x = 0.002$ was used, but since the input functions enter the integral in the combination $S(x/y)$, linear interpolation was used to get the values at abscissa x/y .

RESULTS

The tests of the additive method in the single-unknown case involved taking a test function $S^n(x)$, smearing it with $f_{11}^{n/d}(y, 1)$, and applying the extraction method to the “data” $\tilde{S}^n(x)$ to try to recover the test function. The results of this procedure are shown in Figure 4 for test functions which roughly resemble the expected shape for neutron SFs F_2^n and xg_1^n at $Q^2 = 1 \text{ GeV}^2$. The same procedure was applied to the two-unknown case, with test functions resembling xg_1^n and xg_2^n at $Q^2 = 1.3 \text{ GeV}^2$, and using all four smearing functions $f_{ij}^{n/d}(y, \gamma)$ with the full γ -dependence. The results are shown in Figure 5.

The extraction method was also applied to fits of g_1^d and g_1^p data, from the EG1 experiment in CLAS at TJNAF, by S. Kuhn and N. Guler. The fitting was done using a simplified model of the deuteron as the sum of two free nucleons; this model ignores the corrections represented by the smearing functions, so our extracted neutron function is expected to be heavily model-dependent. For this reason, the extraction was performed neglecting the off-diagonal contribution from f_{12} , which is expected to be quite small compared with the errors inherited from using a simplified fit. The results as shown in Figure 6 are only an illustration of how the method would

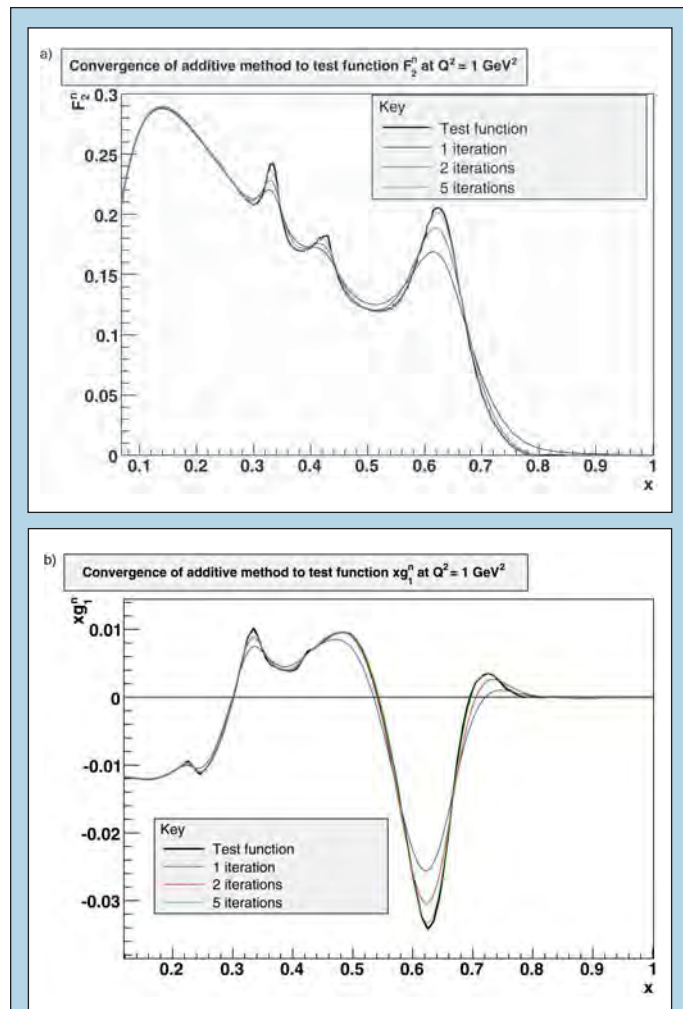


Figure 4. Tests of the additive recursion method (single-unknown case) on test functions (a) F_2^n and (b) xg_1^n , using smearing functions with $\gamma=1$.

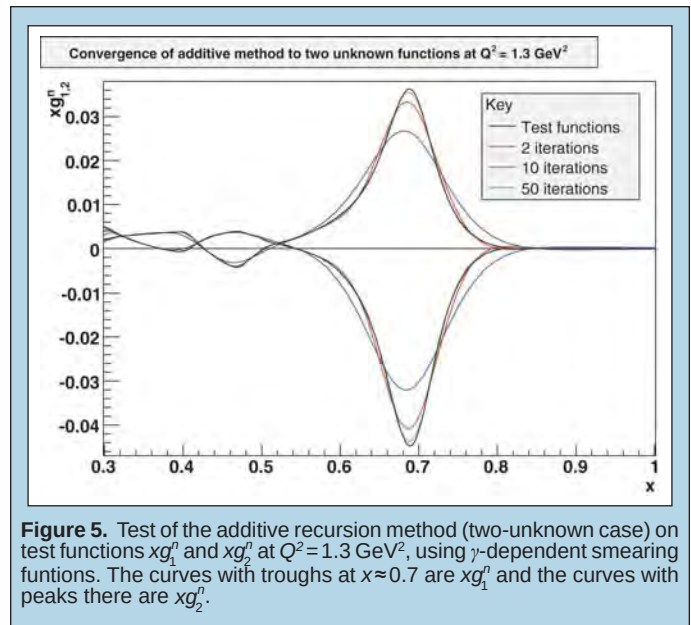


Figure 5. Test of the additive recursion method (two-unknown case) on test functions xg_1^n and xg_2^n at $Q^2 = 1.3 \text{ GeV}^2$, using γ -dependent smearing functions. The curves with troughs at $x \approx 0.7$ are xg_1^n and the curves with peaks there are xg_2^n .

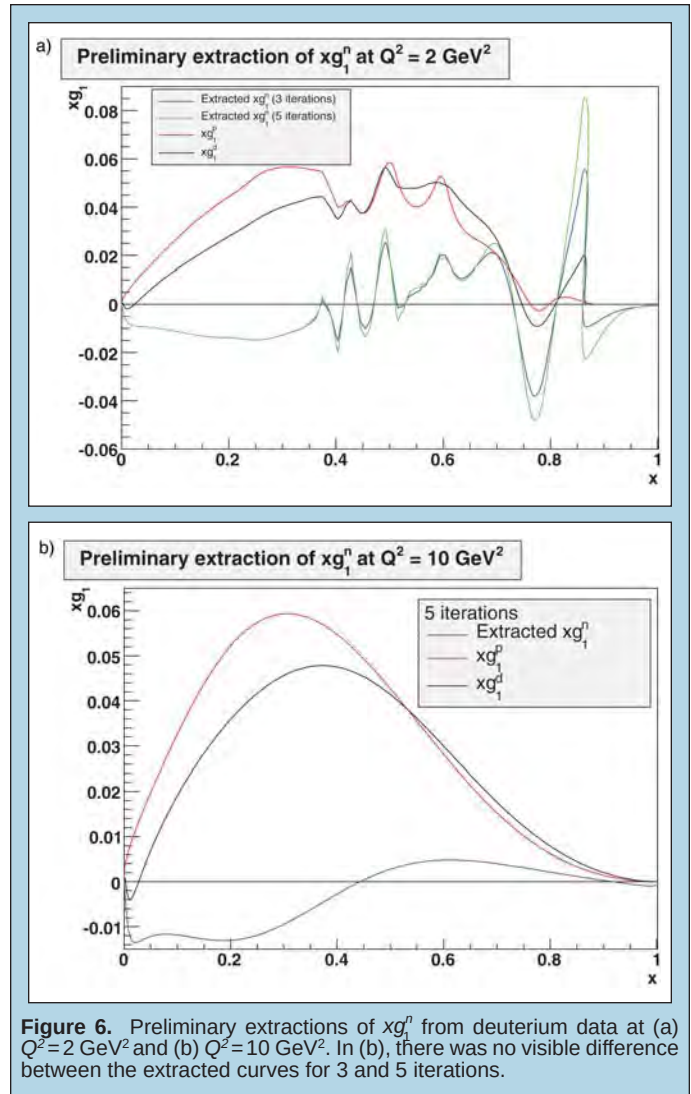


Figure 6. Preliminary extractions of xg_1^n from deuteron data at (a) $Q^2 = 2 \text{ GeV}^2$ and (b) $Q^2 = 10 \text{ GeV}^2$. In (b), there was no visible difference between the extracted curves for 3 and 5 iterations.

be applied to real data. A more detailed analysis, using only the actual data points and including a thorough error estimate, will be performed in future work.

DISCUSSION AND CONCLUSION

The convergence of the additive solution method to test functions in the single-unknown case is clearly illustrated in Figure 4; after only five iterations, the extracted function is nearly indistinguishable from a test function of essentially arbitrary shape. Furthermore, the initial guess for these test functions was $S^{(0)}(x) = 0$, which is quite far from the correct function, so it appears that the effectiveness of this method is nearly independent of the initial guess. To explain these features, write $S^{(0)}(x) = S_{true}(x) + \epsilon^{(0)}(x)$, i.e., the true function $S(x)$ with an error. Tracking this error after one iteration gives

$$\epsilon^{(1)}(x) = \epsilon^{(0)}(x) - \frac{1}{\langle \sigma \rangle} \int_x^{y_{max}} f(y) \epsilon^{(0)}\left(\frac{x}{y}\right) dy. \quad (16)$$

Note that if $f(y) = \delta(y-1)$, the integral in equation (16) is $\epsilon^{(0)}(x)$ as long as $x < 1$, and the error after one iteration vanishes. In fact, since $f_{11}(y, 1)$ is sharply peaked at $y = 1$ (Figure 3), $\epsilon^{(1)}(x)$ is expected to be quite small for $x < 0.8$ regardless of $S^{(0)}$, which is confirmed in Figure 4. This is true except at points x_0 such that $S_{true}(x_0)$ is sharply peaked; the correction term in equation (16) at x_0 will always be too small, since the error $\epsilon^{(0)}$ gets smeared by $f(y)$. Thus, convergence is fastest away from the peaks of $S(x)$. It is rather surprising that the two-unknown case also converges, as demonstrated in Figure 5, even though the off-diagonal functions, f_{12} and f_{21} , no longer resemble delta functions, and the diagonal functions f_{11} and f_{22} spread considerably with increasing x at fixed Q^2 . It may be the case that this procedure converges for *arbitrary* smearing functions, which would provide an alternative numerical solution to Volterra equations of the equation (7) type whose kernels and all higher derivatives vanish along the diagonal.

The results from real data, as noted above, are heavily model-dependent due to the simplified fits of deuterium data used in the analysis. However, a few general features are evident. Discontinuities in the input SF g_1^d and its derivative are amplified in the extracted SF, as can be seen at $x = 0.4-0.5$ and $x = 0.85$ (Figure 6a). Therefore, smooth fits to deuterium SFs are desirable in order to reduce noise in the output. In addition, overshoots such as the one at $x = 0.85$ are seen to grow with increasing numbers of iterations. Such behavior may be explained by the fact that existence and uniqueness of solutions for Volterra equations with vanishing diagonal kernel are no longer guaranteed; there may be no “correct” function to converge to if the LHS of equation (3) is arbitrary, which is the case for data with experimental errors. In this particular case, the overshoot, which is unphysical since the neutron SF has a threshold at the same x value as the proton SF, is caused by ignoring the quasi-elastic peak in the deuteron SF, which begins to dominate the data at $x = 0.85$. A thorough treatment of this correction will be included with a more detailed analysis in future work.

The success of the procedure on test functions suggests that neutron SFs extracted from real data should be reliable within the context of the convolution model. However, one can independently check that the neutron SF satisfies the Bjorken sum rule as follows:

$$I = \int_0^1 (g_1^p - g_1^n) dx = \frac{1}{6} g_A, \quad (17)$$

where g_A is the axial charge of the proton. This test was performed in the DIS region (Figure 6b), where the data parameterizations were smoother and the extraction procedure converged. I in equation (17), was computed for a DIS parameterization [8] and our extraction, cutting the integral off in both cases at $x_{min} = 0.01$ because the extraction of xg_1^n gives no information on the value of g_1^n at $x = 0$. This does not test the Bjorken sum rule per se, which would require the integral of the SFs to extend to $x = 0$, but verifies that the Bjorken integral $\int_{x_{min}}^1 (g_1^p - g_1^n) dx$ has the same value for both a known parameterization and the extracted function. The result from work done by Blümlein and Böttcher [8] was 0.1614, while our result was 0.1695, which is in excellent agreement given that the off-diagonal contribution from f_{12} was neglected.

Despite extensive experiments on light nuclear targets, the neutron remains something of a mystery. While proton observables such as spin-averaged and spin-dependent SFs are known to a high degree of accuracy over a wide range of Q^2 , the corresponding neutron observables are rather poorly constrained, especially in the resonance region. Previously, the low statistics and large errors from experiments designed to measure neutron observables limited the accuracy of measured neutron SFs far more than the simplified model of the nucleus used to perform the extraction. The situation has changed with recent experiments at TJNAF. Accounting for nuclear corrections in neutron SF extraction procedures is now essential to obtain an accurate representation of the neutron SFs. In particular, the finite- Q^2 dependence of the smearing functions, parameterized by γ , is an essential ingredient for obtaining realistic neutron SFs. To assess quark-hadron duality for the neutron to the same extent that it has been verified for the proton, detailed knowledge of all neutron SFs in both the resonance and DIS regions is needed. The method presented in this paper, when applied to the most recent TJNAF data, will be a first step in that direction.

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Kristin Kowolik, originally from Berkeley, CA, graduated from the University of California–Berkeley in 2008 with a B.S. degree in Chemistry. During her Lawrence Berkeley National Laboratory (LBNL)-sponsored SULI internship in the summer of 2008, she traveled to Bangladesh where she conducted research on arsenic removal using electrochemistry. Kristin currently lives in Berkeley and works at LBNL doing research on batteries for hybrid cars. In 2009 she hopes to enter graduate school and work towards a Ph.D. in Chemistry. In her spare time Kristin likes to hike and read books.

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ELECTROCHEMICAL REMEDIATION OF ARSENIC-CONTAMINATED GROUNDWATER — RESULTS OF PROTOTYPE FIELD TESTS IN BANGLADESH

KRISTIN KOWOLIK, SUSAN E.A. ADDY AND ASHOK GADGIL

ABSTRACT

According to the World Health Organization (WHO), more than 50 million people in Bangladesh drink arsenic-laden water, making it the largest case of mass poisoning in human history. Many methods of arsenic removal (mostly using chemical adsorbents) have been studied, but most of these are too expensive and impractical to be implemented in poor countries such as Bangladesh. This project investigates ElectroChemical Arsenic Remediation (ECAR) as an affordable means of removing arsenic. Experiments were performed on site in Bangladesh using a prototype termed “sushi”. This device consists of carbon steel sheets that serve as electrodes wrapped into a cylinder, separated by plastic mesh and surrounded by a tube-like container that serves as a holding cell in which the water is treated electrochemically. During the electrochemical process, current is applied to both electrodes causing iron to oxidize to various forms of iron (hydr)oxides. These species bind to arsenic(V) with very high affinity. ECAR also has the advantage that As(III), the more toxic form of arsenic, oxidizes to As(V) in situ. Only As(V) is known to complex with iron (hydr)oxides. One of the main objectives of this research is to demonstrate the ability of the new prototype to reduce arsenic concentrations in Bangladesh groundwater from >200 ppb to below the WHO limit of 10 ppb. In addition, varying flow rate and dosage and the effect on arsenic removal was investigated. Experiments showed that ECAR reduced Bangladeshi water with an initial arsenic concentration as high as 250 ppb to below 10 ppb. ECAR proved to be effective at dosages as high as 810 Coulombs/Liter (C/L) and as low as 386 C/L (current 1 A, voltage 12 V). These results are encouraging and provide great promise that ECAR is an efficient method in the remediation of arsenic from contaminated groundwater. A preliminary investigation of arsenic removal trends with varying Coulombic dosage, complexation time and filtration methods is also presented.

INTRODUCTION

Arsenic in drinking water is a problem that threatens the lives of close to one hundred million people worldwide. Countries such as Argentina, Chile, Mexico, China and Hungary, as well as some areas of the United States, are severely affected by arsenic-contaminated water. According to the World Health Organization (WHO), in

Bangladesh alone, more than 50 million people drink water that is contaminated with arsenic [1].

Prior to 1970, Bangladeshis were using surface water that was highly contaminated with microorganisms; this led to water-borne diseases especially harmful to children. To address this problem, millions of shallow tube wells were drilled into the Ganges aquifer to gain access to the groundwater and to provide the population with

clean drinking water. It was unknown at the time that arsenic was being introduced into the drinking water due to the dissolution of minerals and ores caused by erosion from local bedrocks [2]. As a consequence, the concentration of arsenic in water in many areas of Bangladesh is 100 times above the 10 ppb limit recommended by WHO [3]. The Bangladeshi government standard for safe drinking water remains at 50 ppb. According to the British Geological Survey (BGS) study conducted in 1998 on shallow tube wells in 61 of 64 districts in Bangladesh, 51% of the wells were above 10 ppb and 27% were above 50 ppb. The survey estimated that the number of Bangladeshis exposed to arsenic concentrations above 50 ppb is 28 to 35 million and the number exposed to more than 10 ppb is 46 to 57 million[4].

Chronic exposure to arsenic through ingestion of contaminated drinking water leads to serious health problems. These include cancers of the lungs, kidney, bladder, urinary tract and skin and cause neurological disease and failure of the kidneys and liver. The appearance of lesions on the feet and hands are effects of longtime exposure to arsenic [5]. In many parts of southern Bangladesh, one in 10 adults is at risk of dying from arsenic-triggered cancers of internal organs [6].

There are several known methods for water purification using the addition of chemical adsorbents that have been implemented in rural areas. These approaches often apply a point-of-use system leaving the operational cost and maintenance to individual families. Consequently, this method leaves a great time burden on Bangladeshis who live on less than one dollar a day. ElectroChemical Arsenic Remediation (ECAR), implements a community-based system that sells clean water at a price affordable to the rural population. ECAR uses electrochemistry to continuously produce Fe(III) ions in solution which quickly hydrolyze, forming iron oxides, hydroxides and/or oxyhydroxides (collectively referred to as iron (hydr)oxides used to remove arsenic (Figure 1)). ECAR is effective, efficient and inexpensive, requiring only very low maintenance. The electrochemical cell consists of two iron electrodes immersed into simulated Bangladesh groundwater. During the electrochemical process, current is applied to the iron anode to form Fe(III) (hydr)oxides while As(III), the more toxic form of arsenic, is simultaneously oxidized to As(V) at the anode. Fe(III) (hydr)oxides

do not bind well to As(III) but have high affinity for As(V) [7]. The iron (hydr)oxides precipitate and coagulate while arsenic adsorbs to the surface, forming insoluble iron-arsenic complexes that can be filtered out using a vacuum filtration system. In the lab, filtration is achieved using a vacuum filter apparatus with a 0.1 micron pore size. Lower cost alternatives are planned for the field, such as simple settling and sedimentation.

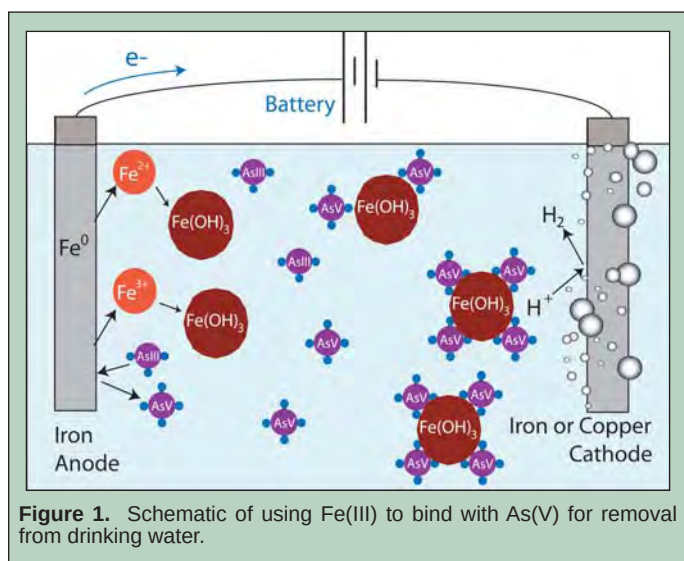
Batch experiments using both simulated and real Bangladeshi groundwater have demonstrated that ECAR is able to reduce arsenic concentration of 600 ppb to less than 10 ppb using current densities between 0.07 and 1.1 mA/cm². Prior lab work has also shown that arsenic removal tends to increase with increasing Coulombic dosage (measured in Coulombs per liter or C/L) and increasing complexation time (defined as the total time of contact between generated iron (hydr)oxides and arsenic contaminants).

The benchtop batch process for ECAR was developed into a continuous flow modular prototype by a team of UC Berkeley students. The device is referred to as “sushi” due to the double roll electrode made from flexible carbon steel foil. It was tested in the laboratory using simulated Bangladesh groundwater, but prior to this work, had never been tested using real groundwater in Bangladesh. Testing with real Bangladesh groundwater is important because the chemical composition in a single well may be different from the composite synthetic groundwater based on average chemical composition across Bangladesh. Differences in chemical composition can potentially have a strong effect on arsenic removal using ECAR.

The primary objective of the prototype field experiments was to demonstrate the ability of the “sushi” prototype to reduce arsenic concentrations in real Bangladesh groundwater from >200 ppb to below the WHO limit of 10 ppb. In addition, spot checks at different Coulombic dosages and complexation times were used to compare general arsenic removal trends to trends in the lab. Also, low cost sedimentation was compared to 0.1 micron vacuum filtration as an alternative method for removing ECAR generated iron-arsenic complexes in the field.

MATERIALS AND METHODS

Arsenic-contaminated water was collected directly at the two wells in the village of Dhingaghanga and stored in 20 L plastic containers that were capped in order to avoid aeration that could lead to oxidation of As(III) to As(V). Prior to water collection, the well was pumped for at least 5 minutes to ensure that the water was coming directly from the aquifer and had not been in contact with the tube well for a long period of time and was free from algae and bacterial contamination. The pH and the dissolved oxygen (DO) of the water was measured and recorded at the field site using a SympHony Ag/AgCl gel-filled combination electrode pH probe and symphony dissolved oxygen probe respectively (VWR International, vwr.com) attached to a portable meter SympHony model SP80PD. To ensure that the collected water contained arsenic, a sample was prepared and tested using a Quick™ Arsenic Test Kit (Industrial Test Systems, Inc, Rock Hill, SC). The test kit contains three reagents that reduce inorganic arsenic to arsine gas. A mercuric bromide test strip is used to measure the arsine gas concentration. It produces a yellow-brown color after exposure to the gas. The test strip is matched to a calibrated color chart in order to obtain a quantitative



measure of arsenic in the water sample. Quick™ Arsenic Test Kit works with highest accuracy if the arsenic concentration is below 100 ppb. If arsenic concentrations are >100 ppb, it is recommended to use a dilution factor.

ECAR treatment was conducted within 120 hours of collection. DO and pH measurements were taken and recorded immediately before the experiment. 100 mL of sample water was filtered through Whatman #1 filter paper to remove particulates that could clog the prototype. The total arsenic concentration was tested using Quick™ Test Arsenic Kit. Some initial portion of the sample was stored for more accurate arsenic measurements via atomic absorption spectroscopy (AAS). The collected water was shaken for five minutes before the experiment. This additional step ensures that all the precipitates that had formed and collected on the bottom of the plastic container between collection at the well head and the ECAR treatment became suspended again in the water matrix.

The “sushi” consisted of two sheets of carbon steel separated by plastic mesh and rolled into a spiral surrounded by a Plexiglas® container that serves as a holding cell in which the water is treated electrochemically. The two sheets of carbon steel serve as the anode and cathode and are connected to a constant current source that provides 1 A with a 12 V car battery used as the power supply. The electrodes dissolve with time and will need to be replaced. Exact lifetime depends on Coulombic dosage required for a given area. The prototype device was attached via tubing to a reservoir that was maintained at 5 L of water at a height of 1 m above the prototype to provide a pressurized inflow. Maintaining a constant water level in the reservoir ensured that the flow rate through the Sushi Roll was constant. The flow rate was adjusted via a valve and set during the first 1 L of flow through the prototype device.

Prototype effluent was stirred on a magnetic stir plate with aliquots removed after 60 and 80 minutes followed by filtration using a Milipore (Billerica, MA) hand-pumped metallic vacuum filter with 47 mm diameter and 0.1 micron Milipore filter membrane. The filtrate was tested for arsenic using Quick™ Arsenic Test Kit. 250 mL of treated water was collected and allowed to settle for 2 days without vacuum filtration. At the end of 2 days settling, one sample was filtered in the manner described above and a second sample was drawn from the top of the sample beaker (no additional filtration).

To ensure more accurate results, samples were sent for Atomic Absorption Spectroscopy (AAS) analysis at BUET, Bangladesh University for Engineering and Technology (Dhaka, Bangladesh). All presented results were obtained by using AAS.

RESULTS AND DISCUSSION

The water used in the experiments was collected from two different wells and the initial total arsenic concentration at the day of the experiment was 200 ppb for Well 7 and 250 ppb for Well 8. All experiments showed very promising results and confirmed that the prototype is capable of reducing the arsenic concentration in groundwater below the Bangladeshi standard of 50 ppb. ECAR was able to reduce the arsenic concentration to below the WHO standard of 10 ppb for both wells under certain conditions (60 minutes stirring at a Coulombic dosage of 810 and 456 C/L for Well 7 and all tested conditions for Well 8).

Figures 2 and 3 present the residual arsenic concentration after ECAR treatment as a function of charge loading (Coulombic dosage in C/L and flow rate in mL/s). Both figures show the results for stirring for 60 and 80 minutes as well as settling for 2 days after electrochemical treatment. The Coulombic dosage was calculated from the measured flow rate and the applied current using the following formula:

$$q = \frac{I}{f}$$

where q = desired Coulombic dosage (C/L), I = current (Amps) and f = flow rate (L/s).

Using the equation above, a flow rate of 1.23 mL/s yields a Coulombic dosage of 810 C/L. With these experimental parameters, the remaining arsenic concentration for Well 7 (initial arsenic concentration is 200 ppb) is 10 ppb after 60 minutes of stirring and 14 ppb after 80 minutes of stirring (Figure 2). A Coulombic dosage of 456 C/L with a flow rate of 2.19 mL/s applied to the same Well 7 water resulted in a remaining arsenic concentration of 8 ppb after 60 minutes and 9 ppb after 80 minutes of stirring (Figure 2).

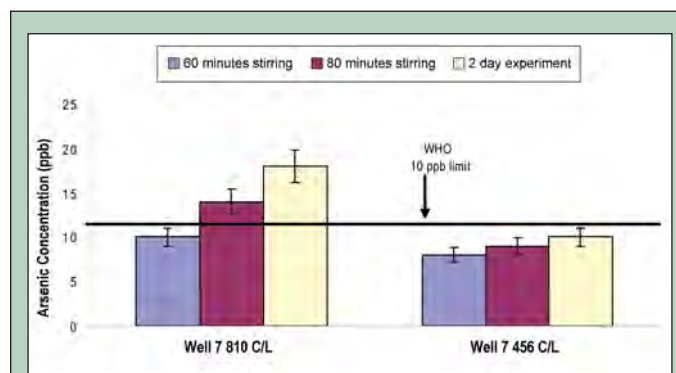
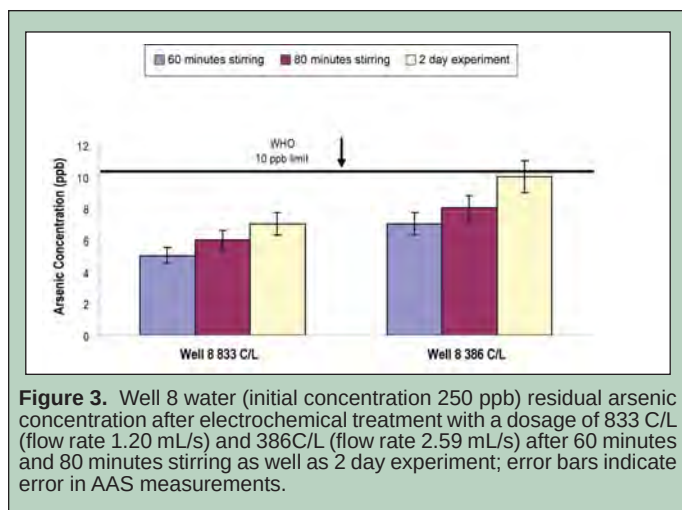


Figure 2. Well 7 water (initial concentration 200 ppb) residual arsenic concentration after electrochemical treatment with a dosage of 810 C/L (flow rate 1.23 mL/s) and 456 C/L (flow rate 2.19 mL/s) after 60 minutes and 80 minutes stirring as well as 2 day settling experiment; error bars indicate error in AAS measurements.

For Well 8 water with an initial concentration of 250 ppb, a Coulombic dosage of 833 C/L and a flow rate of 1.20 mL/s show a residual arsenic concentration of 5 ppb for 60 minutes and 6 ppb for 80 minutes of stirring (Figure 3). A much lower Coulombic dosage of 366 C/L with a flow rate of 2.59 mL/s showed similar results. The remaining arsenic concentration after 60 minutes is 7 ppb and after 80 minutes of stirring it is 8 ppb (Figure 3). In both cases, the trend with decreasing Coulombic dosage was for arsenic removal to stay the same or increase. This trend is different from that seen in the lab (where decreasing Coulombic dosage led to decreasing arsenic removal). More tests are needed to explore the cause of this strange trend.

The 60-minute stirring experiments are most promising. After electrochemical treatment the results showed slightly better residual arsenic concentrations than the 80-minute stirring experiments performed with the same Coulombic dosage and flow rate. Subsequent complexation time during two days of settling showed even less arsenic removal. Possible desorption of arsenic particles during longer stirring time could explain these results. This trend was not observed when similar tests were performed in the laboratory with synthetic water; longer stirring time yielded better results. To better understand these results further experiments are warranted.

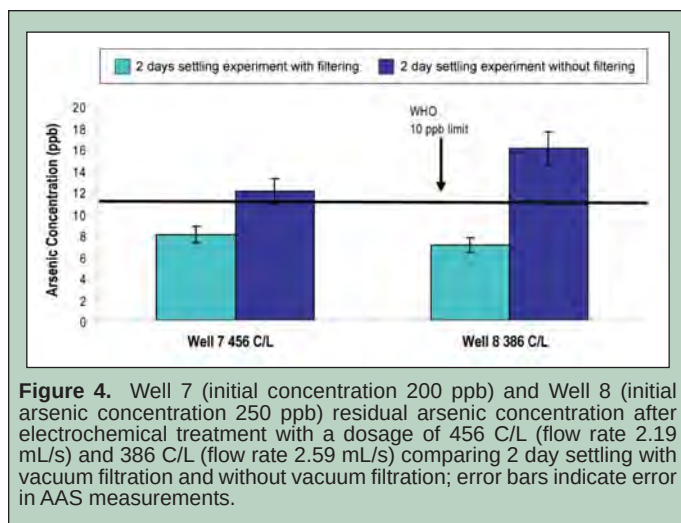


In addition to stirring for 60 and 80 minutes, 250 mL of electrochemically treated water (same Coulombic dosage and flow rate as described above) was set aside for two days and then vacuum filtered and tested for residual arsenic concentration (Figure 2 and 3). A Coulombic dosage of 810 C/L has a residual arsenic concentration of 17 ppb after two days; a Coulombic dosage of 456 C/L has a final arsenic concentration of 9 ppb. Both results are for Well 7 water with an initial arsenic concentration of 200 ppb. The two-day treatment for Well 8 water (initial arsenic concentration is 250 ppb) results in 7 ppb for a Coulombic dosage of 833 C/L and 10 ppb for a Coulombic dosage of 386 C/L. The last result was obtained from Quick™ Arsenic Test Kit (no AAS data was available for this experiment).

Two additional days of complexation time yielded results at or slightly above the WHO standard of 10 ppb. All of the two-day settling experimental results without filtering were below the Bangladeshi standard of 50 ppb, but only the experiments with vacuum filtration had residual arsenic concentrations low enough to be below the WHO standard of 10 ppb. These results suggest that settling and decantation over two days cannot achieve the same arsenic removal as filtration. Some iron-arsenic complexes may still be suspended throughout the water matrix and need to be filtered out in order to ensure a safe final arsenic concentration.

In addition, the two-day settling experiment was also tested for arsenic concentration without a vacuum filter by taking water from the top. These results were then compared to the ones using a vacuum filter (Figure 4). For Well 7 (Coulombic dosage 456 C/L), the residual arsenic concentration is 8 ppb compared to 12 ppb without a vacuum filter. The results for Well 8 (dosage 386 C/L) show 7 ppb with filter versus 16 ppb without vacuum filtering.

The filtered sample of water showed a total arsenic concentration of 281 ppb for Well 7 and 338 ppb for Well 8 whereas the concentrations of the unfiltered water were 200 ppb and 250 ppb, respectively. The above results were measured on the same day. These findings might indicate that arsenic particles bind with the naturally occurring iron ions in the water and are therefore not detected as free arsenic. Filtration may cause the bound arsenic particles to be released from the iron-arsenic complexes and become suspended as free arsenic particles. This behavior is different and has not been observed in the laboratory. Further experimentation is warranted.



CONCLUSION

The objective of testing the “sushi” with real Bangladeshi groundwater was to show that the prototype is efficient in removing arsenic below 10 ppb. The data obtained showed that the device is effective at reducing arsenic concentrations to below 10 ppb from real Bangladesh water at an initial arsenic concentration of >200 ppb.

Spot checks at different Coulombic dosages and complexation times showed trends that were different from those observed in the lab. Results showed that smaller dosage and therefore a faster flow rate works equally as well or even better than a larger dosage and slower flow rate. These findings are encouraging since small dosage and fast flow rate are desirable parameters when turning a prototype into an actual device. However, the fact that the trends are inconsistent with lab trends suggests further study is necessary to make conclusions.

The results indicate that filtration is an essential treatment step that will need to be implemented in the design of a complete device. Using precipitation as an alternative to filtration is an option that needs further investigation. The results have shown that a device including a precipitation step will increase the treatment time by at least two full days.

The device was built as a bench style prototype. The experimental flow rates do not reflect flow rates that will be needed in a scaled-up device. The data obtained help to constrain the parameter space for optimization of flow rate and Coulombic dosage.

One future goal is to test the prototype with arsenic water that has a higher initial concentration (preferably higher than 250 ppb) and perform more detailed studies to determine the cause of arsenic removal trends at various ECAR parameters. These experiments are essential in order to ensure that the device is able to remove arsenic robustly in the field.

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RECONSTRUCTION OF FALSE SPRING OCCURRENCE OVER THE SOUTHEASTERN U.S., 1901–2007: INCREASING RISK OF SPRING FREEZE DAMAGE?

GARRETT P. MARINO AND DALE P. KAISER

ABSTRACT

Near-record warmth over much of the United States during March 2007 promoted early growth of crops and vegetation. A widespread arctic air outbreak followed in early April, resulting in extensive agricultural losses over the southeastern U.S. This “false spring” event also resulted in widespread damage to newly grown tissues of native deciduous forest species, shown by previous researchers to have affected the terrestrial carbon cycle. The current study reconstructed the historical occurrence of false springs for the southeastern U.S. (32–39 °N; 75–98 °W) from 1901–2007 using daily maximum and minimum temperature records from 176 stations in the Global Historical Climatology Network database, and Enhanced Vegetation Index (EVI) data derived from Moderate Resolution Imaging Spectroradiometer (MODIS) satellite observations. A false spring index examined the relative timing of the start of the growing season (SGS), or leaf-out, to the timing of a potentially damaging last hard freeze (≤ -2.2 °C). SGS was modeled for the domain by combining EVI data with ground-based temperature “degree-day” calculations reflecting the rate of springtime warming. No significant area-wide, long-term SGS trend was found (0.2 days later/decade; $p=0.3$). However, the timing of the last hard freeze did occur significantly later (>1 day/decade; $p<0.05$) over a contiguous region stretching from Mississippi eastward to the Carolinas. The index also found that false spring risk increased over the same area, although a domain-averaged trend showed no change since 1901. These results illustrate the complexity of observed climate change over the last century. In a generally warming world, the character of temperature changes in some regions does not result in decreasing risk of false spring, and may in fact pose increased risk if occurring during vulnerable plant growth stages.

INTRODUCTION

Persistent warmth engulfed much of the conterminous United States during March 2007, prompting the early growth of vegetation and of many agricultural and horticultural crops. In early April, a shift in the atmospheric flow pattern brought cold arctic air southward into the central and eastern U.S. This cold air penetrated the region for nearly a week, with temperatures dropping to freezing as far south as the Gulf Coast. Freeze damage was reported in nearly every state from Kansas and Oklahoma east to the Carolinas and Georgia, with estimates indicating total agricultural losses of about two billion dollars [1]. Commodities affected by the arctic air outbreak included winter wheat, emerged corn and blooming fruit trees such as apples and peaches. The 2007 false spring event

also resulted in widespread damage to newly grown tissues of native deciduous forest species. Previous researchers have shown that this damage created both short-term and possible enduring effects on the terrestrial carbon cycle over the southeastern U.S. [2].

The false spring of 2007 should not be considered an isolated event; the literature has documented several similar events over the U.S. (e.g., [3]–[4]). The 2007 event, however, supports the concern expressed by plant ecologists over 20 years ago: a warming global climate could actually increase the incidence of false spring freeze damage to temperate deciduous forests [5]. The area most affected by the 2007 false spring, the southeastern U.S., is an observationally distinctive region where this concern can be tested. Much of the globe has experienced pronounced warming over the past century, as extensively documented in the Intergovernmental

Panel on Climate Change's latest report [6]. In contrast, analysis of annual mean temperatures (T_{ann}) from this part of the globe shows a statistically significant decrease since 1901 (Figure 1; $p = 0.05$) due to a historically unprecedented cool period from the 1960s through the 1980s [7]. The temperature break that occurred in the late 1950s has been noted in the literature and is likely to be real [8].

Due to the character of temperature changes over the southeastern U.S., and due to poorly understood natural variability and regional climate change feedbacks, has risk of false spring freeze damage changed over the same areas affected by the 2007 U.S. spring freeze? To address this question, we developed a model to reconstruct historical trends in false spring occurrence and severity over the southeastern U.S. We diagnosed false springs by comparing the relative timing of the start of the growing season, or leaf-out, to the timing of a potentially damaging last hard freeze ($\leq -2.2^\circ\text{C}$, or $\leq 28^\circ\text{F}$). Leaf-out signals the beginning of the photosynthetic season and influences subsequent carbon cycling and productivity [9]. Regional long-term networks of phenology, i.e., the study of annually recurring events such as leaf-out, are currently sparse and temporally limited [10]. Therefore, we generated an empirical phenology model that integrated remotely sensed phenology from satellite data with surface weather records. This approach offered improvements over recent attempts in the meteorological literature to define the start of the growing season [11]–[13]. The model, albeit imperfect, offered an attractive advantage: it allowed for reconstructions of phenology (and consequently false springs) back through the instrumental weather record, providing a context for the more recent and limited satellite data.

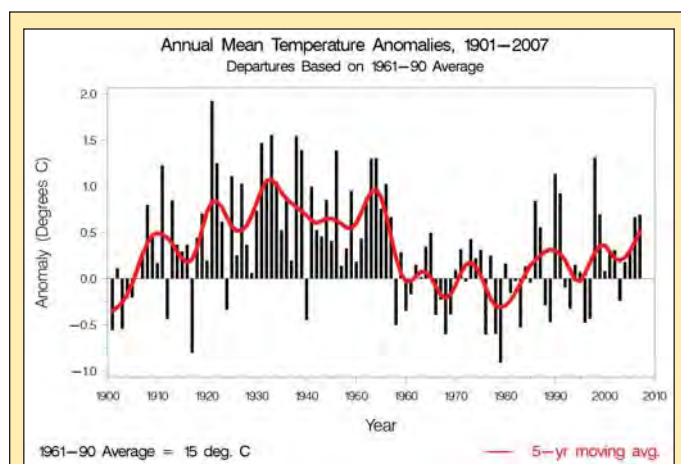


Figure 1. Annual mean temperature anomalies for the southeastern United States from 1901–2007. Anomalies are calculated using a 1961–90 base period, with positive anomalies indicating warmer conditions. The red line is a smoothed 5-year central moving average. Temperatures have significantly decreased since 1901 ($-0.36^\circ\text{C}/\text{century}$; $p = 0.05$), although over the past 50 years that trend has significantly reversed ($+0.99^\circ\text{C}/\text{century}$; $p = 0.03$).

METHODS

Meteorological Data

A common limitation of studies examining extreme meteorological events (such as false springs) is their use of data beginning during the mid-twentieth century (e.g., [14]), mainly due to the absence of digitally available daily data. Recent efforts to digitize and quality assure surface weather records stretching

back to the nineteenth century [15], [16] have resulted in an enhanced set of daily temperature and precipitation data for many regions of the globe. For this study, daily maximum and minimum temperature observations from 1901–2007 for 309 stations over the southeastern U.S. ($32\text{--}39^\circ\text{N}$; $75\text{--}98^\circ\text{W}$) were extracted from the Global Historical Climatology Network database (GHCN) [17]. These data have undergone quality assurance checks at the National Climatic Data Center (NCDC). The spatial domain was chosen to include the forested and agricultural areas most affected by the false spring of 2007. To ensure high data quality, station records were analyzed for temporal gaps, missing data and NCDC-assigned quality flags. Stations were kept if fewer than 20 years between 1901–2007 exhibited quality problems, missing no more than five consecutive years at any point. These selection criteria narrowed the number of stations to 176 for further data processing and analysis.

Model for the Start of the Growing Season

The occurrence and severity of false springs depends on the relative timing of the start of the growing season (SGS), or leaf-out, to the timing of a potentially damaging last hard freeze ($\leq -2.2^\circ\text{C}$, or $\leq 28^\circ\text{F}$). We introduce a false spring index (FSI) that considers these two influences and resembles indices mentioned in the literature ([11], [18]). A positive FSI value indicates a likely false spring, with damage to crops and vegetation.

$$FSI = \text{Day of year (last hard freeze)} - \text{Day of year (SGS)} \quad (1)$$

Determining SGS in the index requires an empirical model because extensive multi-species phenological data are currently limited for the United States, and therefore no direct measurement of SGS can be implemented back to 1901. Here, a simple model of the approximate timing of leaf-out is employed to reconstruct SGS over the period of record, 1901–2007. The model combines Enhanced Vegetation Index (EVI) data derived from Moderate Resolution Imaging Spectroradiometer (MODIS) satellite observations with a ground-based temperature “degree-day” approach reflecting the rate of springtime warming. Remote sensing products like EVI have been used to monitor plant growth stages [19], and are related to the column integral of chlorophyll in the canopy [20]. Twelve deciduous forest sites in or near the domain were selected for the model (see Table 1), and available EVI data from 2000–2008 for these locations were extracted from the MODIS land subsets online interface [21] and the MODIS/Terra Vegetation Indices 16-Day L3 Global 250m SIN grid V005 (MOD13Q1) product [22]. The locations were selected based on several considerations and represent a range of forest species: the subset location must have a discernible annual EVI cycle, be within 25 miles of a meteorological reporting station of similar elevation (< 250 ft. absolute elevation difference), and contribute to a good spatial coverage of the domain (no stations closer than 50 miles to one another). The two coldest sites in Pennsylvania and Ohio were selected, despite being outside of the domain, to ensure that the phenology model could be extended to the coldest sites in the GHCN dataset (5 of 176 GHCN sites have an annual mean temperature [T_{ann}] between 9.6 and 12.0°C). The T_{ann} range for all GHCN stations was 9.3°C ($9.6\text{--}18.9^\circ\text{C}$).

Deciduous forest sites were chosen because they comprise the majority of the domain [19], and agricultural areas (mainly winter wheat) are concentrated in the western regions. SGS was then defined as the date in late winter or early spring when the site's EVI

pixel value exceeded four standard deviations of its December-to-early-February winter baseline, corresponding to about two standard deviations above uncertainties associated with a larger 7x7 pixel grid centered at the point considered. Due to the small sampling frequency of the available satellite data (one EVI value for each 16-day period), and inherent EVI measurement error, the uncertainty associated with the satellite-derived SGS was about one week for most cases. To determine SGS, a linear interpolation was used between sequential EVI values. An assumption of the SGS definition was that the majority of crops would be vulnerable to hard freezes by the timing of SGS, which is reasonable upon considering the 2007 false spring. The SGS definition thus provides an approximate measure of both vegetative and agricultural development.

After SGS was established at the MODIS subset locations, Local Climatological Data [23] from nearby surface weather stations were extracted and growing degree-day (GDD) units were accumulated from a beginning base date (March 1) to the satellite-derived SGS date for each site-year. The base daily mean temperature for the GDD calculations was 10 °C, a typical value used in the literature [24]. That is, if a daily mean temperature exceeded 10 °C, then the difference between the actual and base temperatures was taken as the day's GDD contribution. This method enabled GDD thresholds to be implemented on the historical GHCN data to reconstruct SGS over the domain since 1901.

RESULTS

Start of the Growing Season

We first plotted the average MODIS-derived SGS for each of the 12 subset sites versus their respective annual mean temperature (T_{ann}) and found a strong linear relationship ($r^2=0.91$). This result suggests that temperatures may explain a large portion of SGS variance and supports the use of GDD thresholds to define SGS.

The average GDD threshold for each subset site is given in Figure 2, along with $\pm 1 \sigma$ variability. A linear best-fit relationship with T_{ann} explains 66% of the variance in GDD, and generally works well for all the sites:

$$GDD = 4.77 (T_{ann}) + 36.81 \quad (2)$$

Furthermore, this best-fit model predicts SGS dates only 0.2 (± 5.0) days later than the satellite observations, with a range of -12 to 10 days for all site-years. Equation (2) is used to reconstruct SGS back to 1901. A station's T_{ann} is the only parameter needed to define the GDD threshold and consequently SGS for each year and location across the domain. A result we find later is that long-term station trends in SGS are not sensitive to the GDD threshold employed, but Equation (2) provides calibrated SGS values.

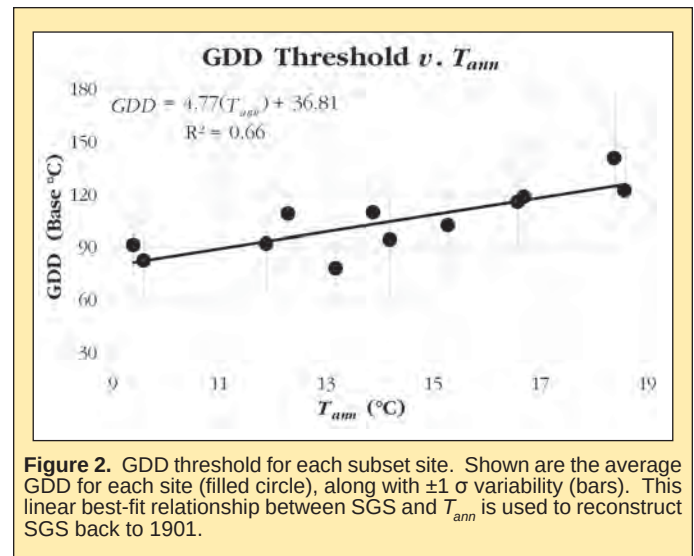


Figure 2. GDD threshold for each subset site. Shown are the average GDD for each site (filled circle), along with $\pm 1 \sigma$ variability (bars). This linear best-fit relationship between SGS and T_{ann} is used to reconstruct SGS back to 1901.

Modis Subset Location	Nearby Weather Station	Weather Station, T_{ann} (°C) ^a
Penn State SURFRAD Station, PA	State College, PA	9.4
Oak Openings, OH	Toledo Express Airport, OH	9.6
Morgan Monroe State Forest, IN	Bloomington Indiana University, IN	11.9
Missouri Ozark Site, MO	Columbia Regional Airport, MO	12.3
Asheville 8 SSW — North Carolina Arboretum (Bierbaum Site), NC	Asheville Regional Airport, NC	13.2
Bowling Green 21 NNE — Mammoth Cave National Park, KY	Bowling Green-Warren County Regional Airport, KY	13.9
Walker Branch Watershed, TN	Oak Ridge, TN	14.2
Duke Forest — Hardwoods, NC	Raleigh-Durham International Airport, NC	15.3
Goodwin Creek, MS	Batesville 2 SW, MS	16.6 ^b
Watkinsville 5 SSE — USDA/ARS (Colham Ferry Site), GA	Athens Airport, GA	16.7
Monroe 26N — Upper Ouachita National Wildlife Refuge, LA	Monroe Regional Airport, LA	18.4
Selma 13 WNW — Auburn, AL	Selma, AL	18.6

^a Based on 1971–2000 data.

^b T_{ann} from nearby Charleston, MS.

Table 1. MODIS subset sites and locations of nearby weather stations with their T_{ann} .

Upon applying Equation (2) to the GHCN station data, we find that T_{ann} accounts for 98% of the variance in SGS (Figure 3b). The strong linear relationship found here also falls within the 95% confidence interval of a similar model derived from surface tower observations of ecosystem CO_2 exchanges [9, Figure 3].

Figure 3 also illustrates a color-coded dot map of the average SGS date for every station in the domain (Figure 3a). Also shown is a map of SGS trends for each station spanning 1901–2007 (Figure 3c), supplemented by a time series of the domain-averaged SGS values (Figure 3d). Results indicate that despite the large interannual variability of the modeled SGS, there exists no significant long-term trend over the domain (0.2 days later/decade, $p=0.3$).

Timing of the Last Hard Freeze

The timing of the last hard freeze ($\leq -2.2^\circ\text{C}$) represents the second part of the false spring index [FSI; Equation (1)], introduced to assess historical changes in false spring occurrence over the domain. About 92% of the variance in the last hard freeze date can be accounted for by T_{ann} (Figure 4b), further evidence that T_{ann} is the dominant factor, on an average, determining annually recurring events such as SGS and last freeze. Additional results (Figure 4d) indicate that the domain-averaged last hard freeze date has not significantly changed since 1901. However, the last hard freeze occurred significantly later (>1 day/decade) over a contiguous region stretching from Mississippi eastward to the Carolinas, while areas to the northwest exhibited the opposite trend (Figure 4c).

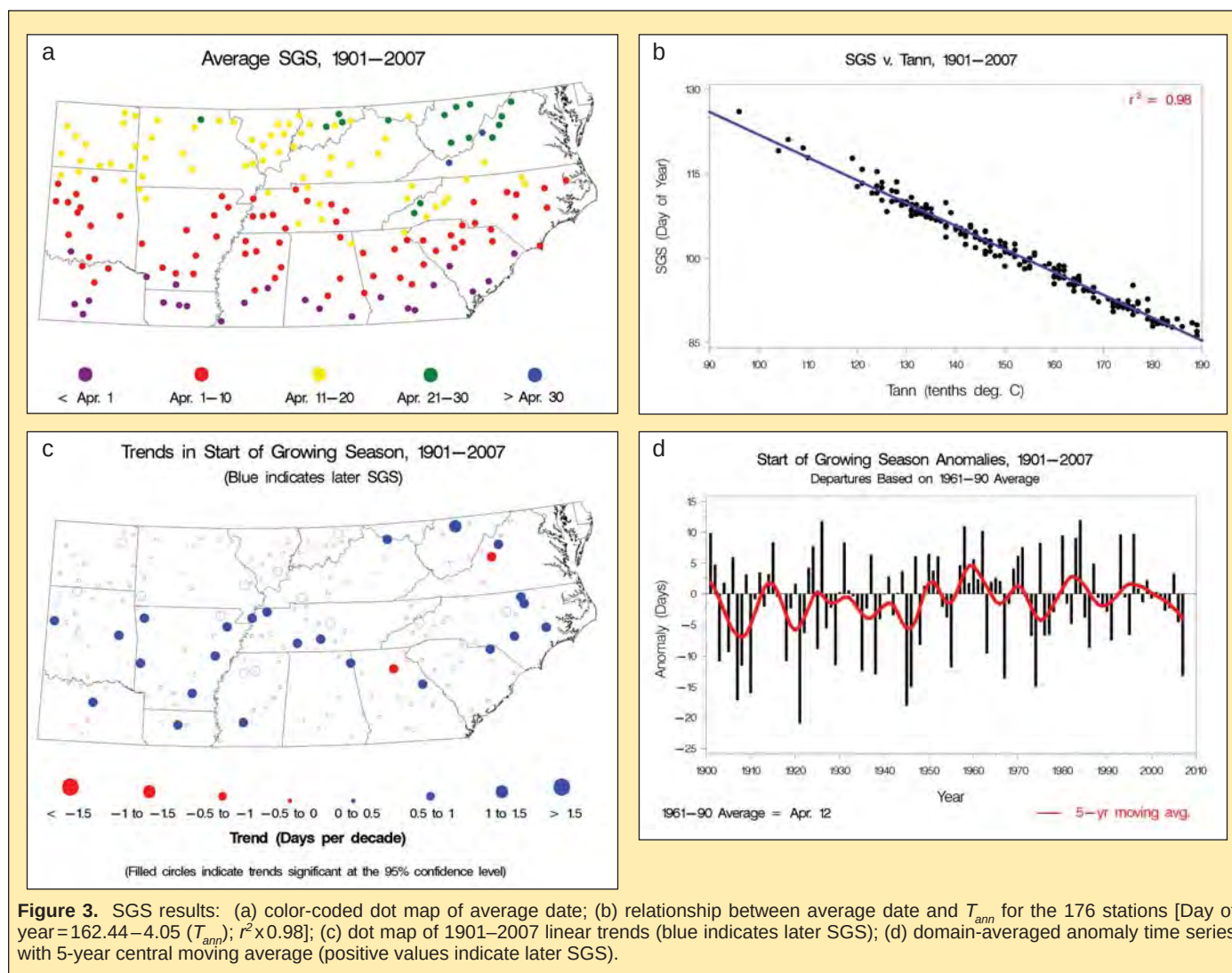
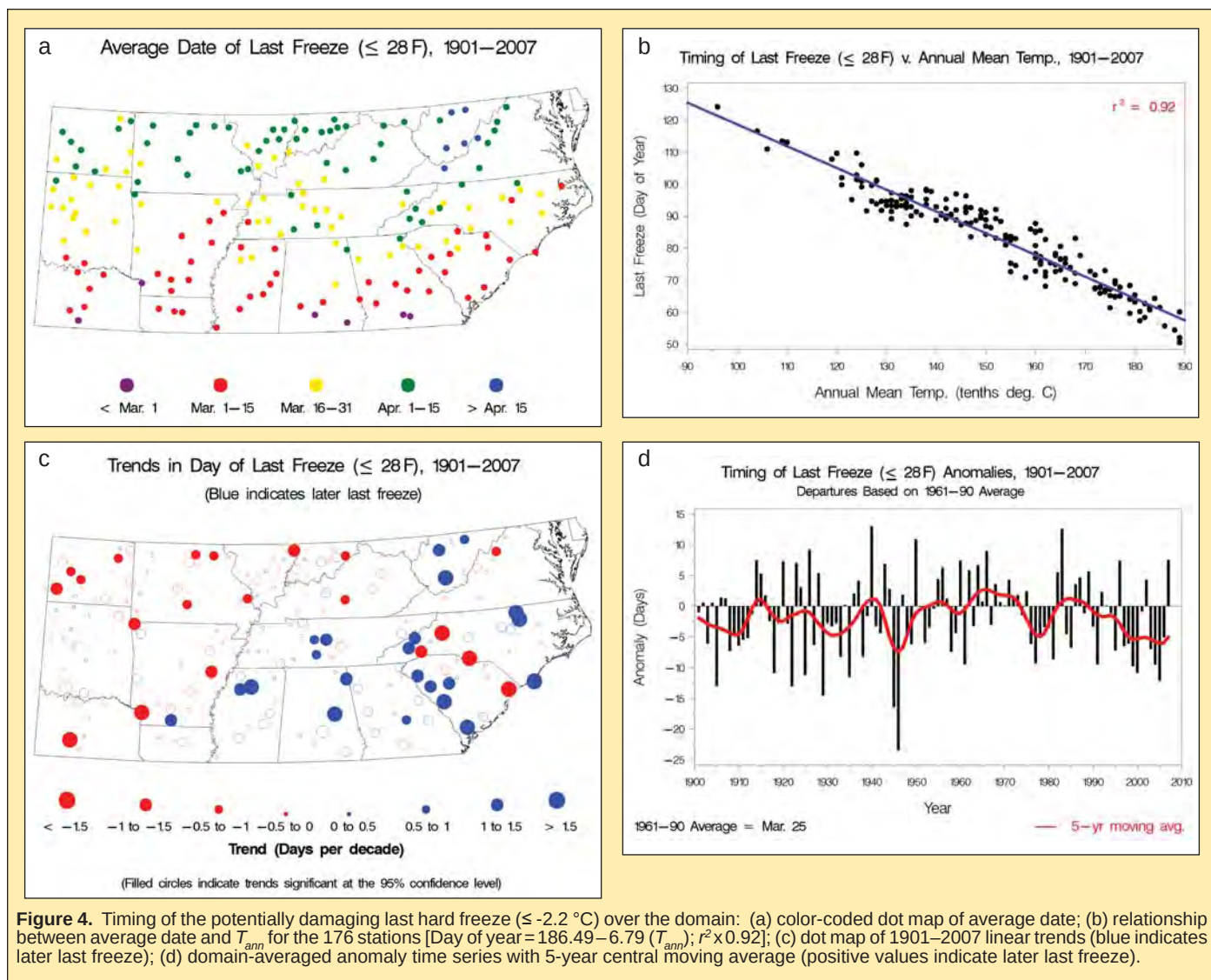


Figure 3. SGS results: (a) color-coded dot map of average date; (b) relationship between average date and T_{ann} for the 176 stations [Day of year = $162.44 - 4.05 (T_{ann})$; $r^2 = 0.98$]; (c) dot map of 1901–2007 linear trends (blue indicates later SGS); (d) domain-averaged anomaly time series with 5-year central moving average (positive values indicate later SGS).



False Spring Index

The false spring index considers the relative timing of SGS to the last potentially damaging hard freeze. A domain-averaged FSI trend (Figure 5d) shows no change in risk of false spring since 1901. The FSI captures the false spring of 2007 as the most widespread event over the period of record, although the results suggest several similar events have occurred during the past century, namely in 1907, 1921 and 1955. Spatial trends (Figure 5c) reveal that the contiguous area covering Mississippi eastward to the Carolinas generally exhibited increasing risk of false spring (FSI increasing by 1 day/decade), while areas to the west show reduced risk. A literature search uncovered that the FSI accurately identifies false spring events dating back to 1907 ([4], [25]–[26]).

Figures 5a and 5b reveal a potential shortcoming of the index when applied to cool locations. The coldest stations have average FSI values around -5 days. Either the model does not work well for these locations, or more likely, the damaging threshold temperature at these locations is below -2.2°C . Therefore, an alternative to looking at FSI trends and time series may be to consider the lowest minimum temperature attained after SGS.

The results (Figure 6) are largely consistent with those found using the FSI. Trends show minimum temperatures after SGS decreased over the Gulf States and increased elsewhere. To examine the southern states (MS, AL, GA and SC) more carefully, we computed the minimum temperature after SGS for just those areas in Figure 7.

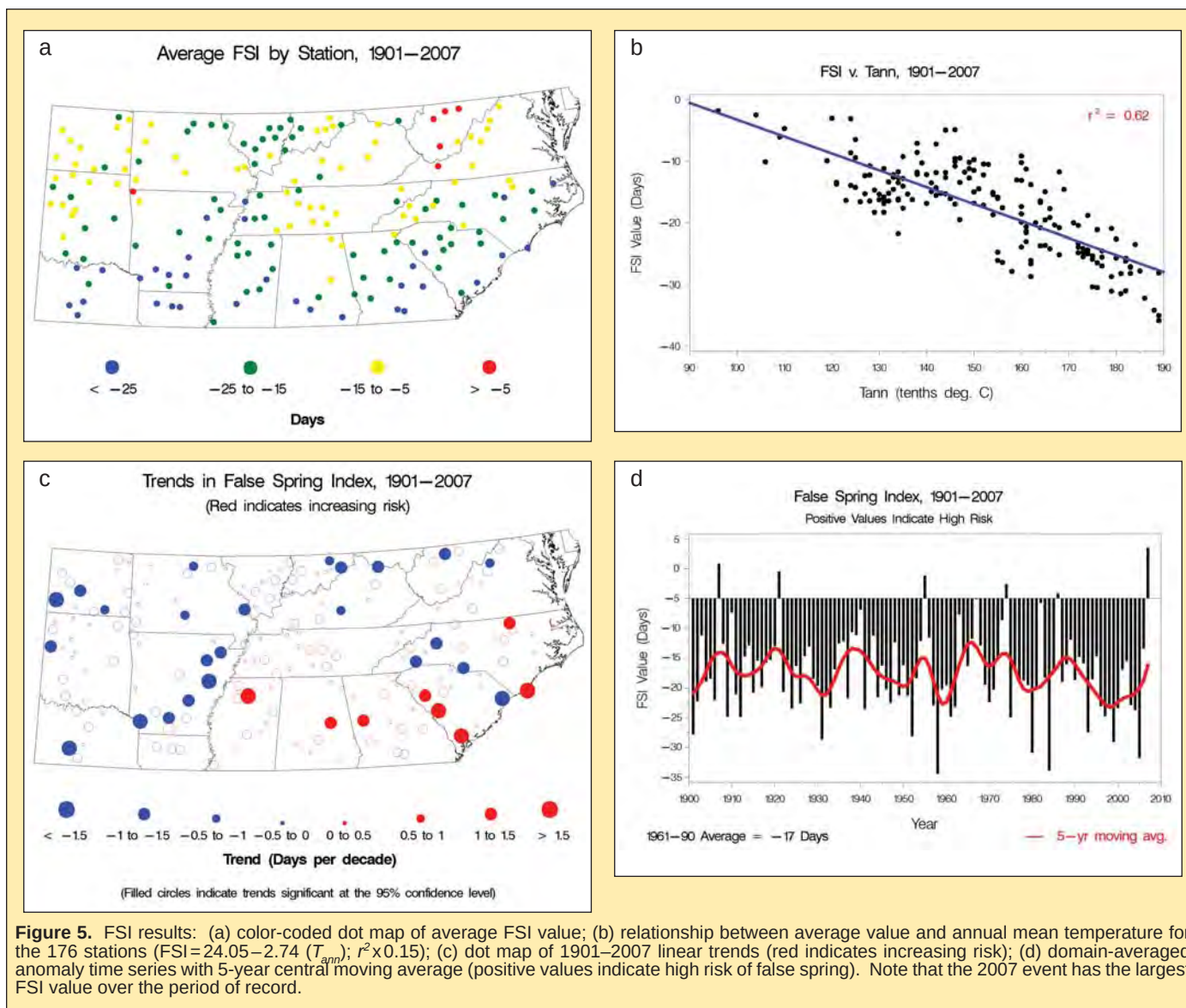


Figure 5. FSI results: (a) color-coded dot map of average FSI value; (b) relationship between average value and annual mean temperature for the 176 stations ($FSI = 24.05 - 2.74 (T_{ann})$; $r^2 = 0.15$); (c) dot map of 1901–2007 linear trends (red indicates increasing risk); (d) domain-averaged anomaly time series with 5-year central moving average (positive values indicate high risk of false spring). Note that the 2007 event has the largest FSI value over the period of record.

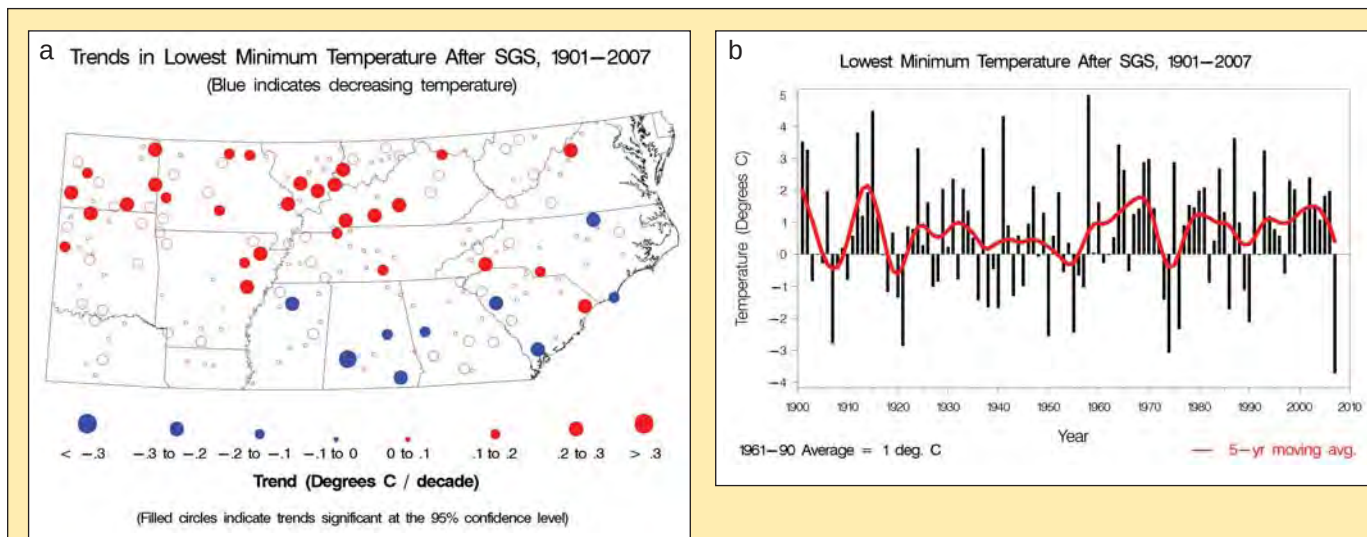
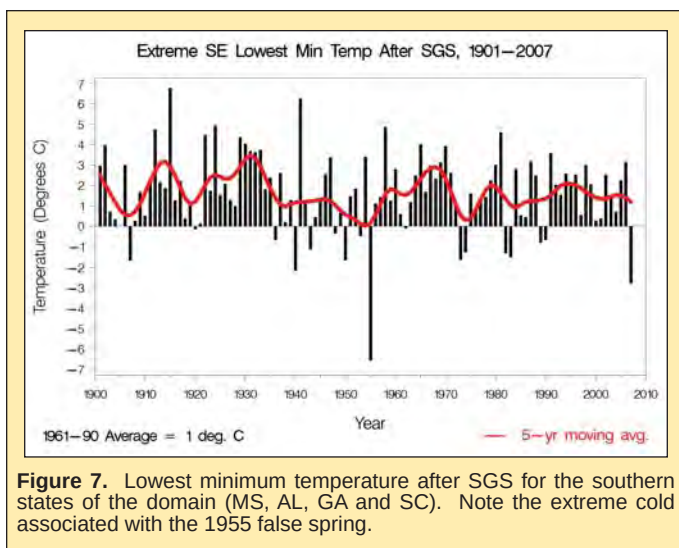


Figure 6. Lowest temperature after SGS: (a) dot map of 1901–2007 linear trends (blue indicates decreasing temperature); (b) domain-averaged anomaly time series with 5-year central moving average (positive values indicate warmer conditions). Note that the false spring of 2007 has the largest negative anomaly in (b).



A different time series emerges by only looking at the southern states. We can clearly see the 2007 false spring, but now 1955 stands out with extreme cold temperatures 4 °C lower than in 2007. A *Monthly Weather Review* article [4] overviews the synoptic situation leading to this damaging cold snap. When looking back at the original FSI time series (Figure 5d), we note that 2007 still appears as a greater anomaly than the year 1955. This could be from either the model not accurately predicting SGS across a large portion of the domain during March 1955, or perhaps more likely that SGS had just started in the southern states when the extreme cold wave occurred, and therefore damage was confined to this region.

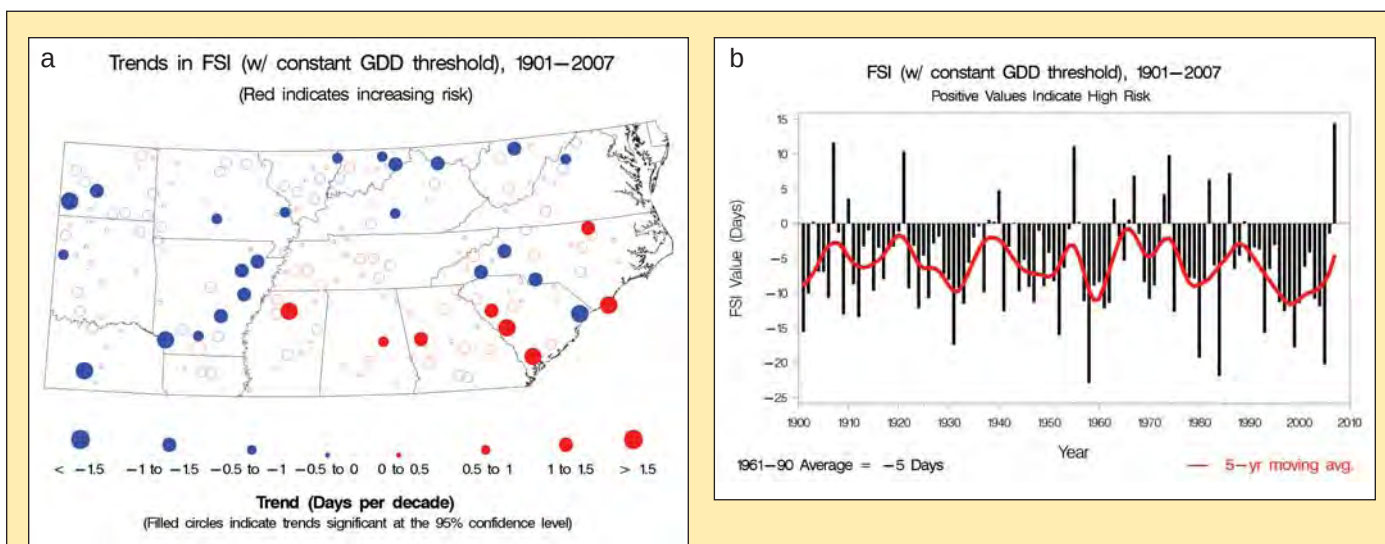
Another important result mentioned earlier is that FSI trends are largely invariant to the GDD definition used to reconstruct SGS. For example, if GDD were kept constant at 100 °C for all site-years (an approximate average of Equation (2)), FSI trends would be nearly indistinguishable from the original results (compare Figure 8a to Figure 5c). However, unrealistic values of FSI resulted from this change (Figure 8b). On the other hand, future identification of the top false spring events will not change.

DISCUSSION AND CONCLUSION

The historical occurrence and severity of false springs over the southeastern United States from 1901–2007 was diagnosed by examining the relative timing of the start of the growing season (SGS), or leaf-out, to the timing of a potentially damaging last hard freeze (≤ -2.2 °C). SGS was accurately reconstructed for the domain by integrating surface temperature records with EVI data derived from MODIS satellite observations. Other studies [29] fail to find a parameterization for their phenology (SGS) models; domain and station volume differences may explain why the same conclusions do not extend to this work. If MODIS subset data were analyzed for every station in the domain, a larger variability would likely exist than in the 12 sites considered here. However, since we are concerned with long-term trends, results suggest that the SGS model is adequately calibrated by the sites examined in this study. We found that the interannual variability of the modeled SGS was large, and no significant area-wide, long-term trend existed. However, SGS has been arriving earlier over a large portion of the globe in recent decades (e.g., [27]–[28]). The southeastern U.S. represents an observationally distinctive land area not following global trends for many climatic variables.

The timing of the last hard freeze was also unchanged over the domain on average, although regionally a contiguous area stretching from Mississippi eastward to the Carolinas experienced a significantly later last freeze while areas to the north and west exhibited earlier dates. Again, the behavior of the extreme Southeast with respect to this variable does not match that of other regions [30]. Risk of false spring was also found to be increasing over the southern states, while a Southeast-averaged trend showed no change in risk since 1901 due to decreasing risk over the region's western and northern areas. Continued observation of the false spring index would be useful to monitor changes in risk.

The findings illustrate the complexity of observed climate change over the last century. In a generally warming world, the character of temperature changes in some regions does not result in decreasing risk of false spring, and may in fact pose increased risk if a false spring occurs during vulnerable plant growth stages.



This work stresses the important need of climate change research to further examine sensitivity of ecosystems to small changes in spring climate, and to better understand large-scale atmospheric circulation modes that can substantially specify regional temperatures and climatic variability. Climate change may not only produce an increase in average temperatures throughout the globe, but may also increase temperature variance [31]. Vegetation development may be sensitive to these larger intra-annual temperature fluctuations, and these fluctuations will influence false spring occurrence. Global-scale plant phenology networks should also be expanded to strengthen understanding of phenological dependence on environmental factors. Ultimately, a SGS model should assimilate these phenology records with satellite and surface weather observations for maximum effectiveness.

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COMPARISON OF SODIUM AND POTASSIUM CARBONATES AS LITHIUM ZIRCONATE MODIFIERS FOR HIGH-TEMPERATURE CARBON DIOXIDE CAPTURE FROM BIOMASS-DERIVED SYNTHESIS GAS

JESSICA L. OLSTAD AND STEVEN D. PHILLIPS

ABSTRACT

The process of gasification converts biomass into synthesis gas (syngas), which can be used to produce biofuels. Solid-phase sorbents were investigated for the removal of CO₂ from a N₂/CO₂ gas stream using a CO₂ concentration similar to that found in a biomass gasification process. During the gasifying process, large amounts of carbon dioxide (CO₂) are created along with the syngas. The produced CO₂ must be removed before the syngas can be used for fuel synthesis and to avoid the possible formation of unwanted byproducts. A thermogravimetric analyzer was used to test the CO₂ absorption rates of sorbents composed of lithium zirconate (Li₂ZrO₃), as well as mixtures of Li₂ZrO₃ with potassium carbonate (K₂CO₃) and sodium carbonate (Na₂CO₃). The experimental results show that Li₂ZrO₃ has a low absorption rate, but sorbents containing combinations of Li₂ZrO₃ and the K₂CO₃ and Na₂CO₃ additives have high uptake rates. Using different proportions of K₂CO₃ and Na₂CO₃ produces varying uptake rates, so an optimization experiment was performed to obtain an improved sorbent. The CO₂ absorption and regeneration stability of the solid-phase sorbents were also examined. A sorbent composed of Li₂ZrO₃ and 12.1 weight % Na₂CO₃ was shown to be stable, based on the consistent CO₂ uptake rates. Sorbents prepared with Li₂ZrO₃, 17.6 weight % K₂CO₃ and 18.1 weight % Na₂CO₃ showed instability during regeneration cycles in air at 800 °C. Sorbent stability improved during regeneration cycles at 700 °C. Further testing of the Li₂ZrO₃ sorbent under actual syngas conditions, including higher pressure and composition, should be done. Once the optimum sorbent has been found, a suitable support will be needed to use the sorbent in an actual reactor.

INTRODUCTION

High energy and transportation costs have increased interest in the thermochemical conversion of biomass into biofuels. Biomass is converted through the processes of gasification, the water-gas shift reaction (CO+H₂O↔CO₂+H₂), and synthesis reactions to liquid fuels. Each of these processes produces carbon dioxide (CO₂) which can negatively impact the system operation. The surplus CO₂ continues through such processes, requiring additional equipment and energy to process. For some synthesis catalysts, excess CO₂ affects the fuel synthesis chemistry. High levels of CO₂ can be an inhibitor to certain synthesis catalysts, reducing the rate of reaction and producing unwanted byproducts. Therefore, it is usually necessary to remove CO₂ from the process to achieve acceptable concentrations of desirable products in the syngas [1].

A common method for removing CO₂ is the use of an aqueous amine scrubbing system. Although the amine absorption system

is typical, it is quite expensive. The chemical absorption process requires the alkanolamine absorbent to be in a liquid phase aqueous solution; the amine liquids are mixed with water to produce specific concentrations that work best under different operating conditions. Once the CO₂ is absorbed into the aqueous amine mixture, it is released in another location by increasing the temperature and decreasing the pressure. This process is energy intensive because the aqueous amine must undergo a phase change from liquid to vapor. Due to water's large heat of vaporization, a significant amount of heat is required for it to boil [2]. This energy expense is the source of a large penalty on process efficiency.

In recent years, there has been an increase in research of solid-phase sorbents for CO₂ capture from flue gases. Researchers have done experiments on numerous types of sorbents to determine whether using solid sorbents is a plausible and economical way of removing CO₂ from fossil fuel plants' emissions. However, the syngas stream in a syngas-to-fuel process is significantly different

than combustion flue gases; syngas has essentially no oxygen (O₂) and very little nitrogen (N₂), and may be at a higher pressure depending on the location in the process from which it is removed. Thus, sorbents shown to be appropriate in flue gas studies may not be effective under syngas conditions.

The use of lithium zirconate (Li₂ZrO₃) as a CO₂ sorbent is becoming increasingly popular. This is due to the high selectivity between CO₂ and N₂, as well as the relatively low regeneration temperature. Ida, et al. [3] obtained positive results after testing several Li₂ZrO₃-based variations under diverse flue gas conditions. It was found that a mixture of Li₂ZrO₃ and potassium carbonate (K₂CO₃) had better sorption properties than Li₂ZrO₃. They concluded that the formation of a lithium carbonate (Li₂CO₃)/K₂CO₃ eutectic liquid improved the diffusion rate of CO₂ from the particle surface to an inner core of Li₂ZrO₃ that becomes increasingly separated from the surface by a shell of ZrO₂ that forms concomitantly with Li₂CO₃ formation.

In our study, several pure and modified Li₂ZrO₃-based sorbents were prepared to test CO₂ sorption performance under typical syngas conditions (excluding higher pressures). The sorption experiments were conducted in a thermogravimetric analyzer at diverse conditions, depending on the sorbent. The performance of each sorbent was based on the rate of sorption for the first 20 minutes of an uptake cycle.

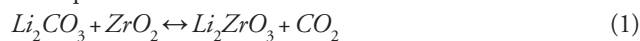
MATERIALS AND METHODS

Each sorbent's ability to uptake CO₂ was tested using a Cahn TG-131 thermogravimetric analyzer (TGA). Each sorbent was placed in the TGA and tested at distinct conditions which influence the overall uptake or release of CO₂ within the sample. The uptake of CO₂ was based on the change in mass of the sample during the experiment. The mass changes were assumed to only be the gain or loss of CO₂ from the sample and the uptake rates for the first 20 minutes of an uptake cycle were reported.

The sorbents that were tested were Li₂ZrO₃, Li₂ZrO₃ doped with potassium carbonate (K₂CO₃), Li₂ZrO₃ doped with sodium carbonate (Na₂CO₃) and Li₂ZrO₃ doped with varying ratios of both additives.

Sorbent Preparation

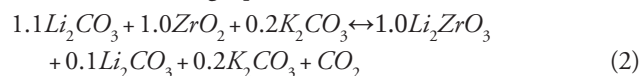
The following sorbent preparations were based on procedures discussed by Pannocchia et al. [4]. Li₂ZrO₃ was made by combining 99+% A.C.S. reagent grade Li₂CO₃ (from Sigma-Aldrich), and 99% metals basis ZrO₂ (from Aldrich), in a 1:1 molar ratio in accordance with the equation:



Enough acetone to make a slurry was mixed in to allow for a more even distribution of the compounds; the mixture was then calcined in air for 6 hours at 850 °C. The temperature increase and decrease rates were 1 °C/min. After calcination, the mixture was ground into a powder and collected for later use.

Two methods were used to dope Li₂ZrO₃ with K₂CO₃.

Method 1: anhydrous K₂CO₃ (from J.T. Baker) was ground into a powder using an agate mortar. The K₂CO₃ was mixed with specified amounts of Li₂CO₃ and ZrO₂. The molar ratios used were taken from the following equation.



The doped mixture was prepared using the same procedure as described for Li₂ZrO₃.

Method 2: Li₂ZrO₃ was made using the initial method, but with the molar ratio changed to 1.1:1.0 moles of Li₂CO₃ to ZrO₂. After the calcination process, the Li₂ZrO₃ was ground and weighed. The quantity of K₂CO₃ needed to give 1.1:1.0:0.2 molar ratio was calculated, and the correct amount of K₂CO₃ was mixed in with the Li₂ZrO₃.

The sample of Li₂ZrO₃ doped with Na₂CO₃ was prepared via method 2, exchanging K₂CO₃ with Na₂CO₃.

The samples containing both K₂CO₃ and Na₂CO₃ were made using method 2. The foundation of each sample was 1 g of Li₂ZrO₃, and the relative amounts of each additive were based on weight ratios rather than molar ratios.

Experimental Procedure

Each initial sorbent sample was tested at various conditions (Table 1). This allowed for the observation of varying affects that each set of conditions would have on the sorbent and established a set method for future testing.

To determine the optimum ratio of K₂CO₃ and Na₂CO₃ for CO₂ absorption, a fixed method was used (Table 2). The sorbent samples tested had a mass of approximately 95 mg. The sorbents were heated in a CO₂/N₂ gas mixture to 800 °C at a ramp of 15 °C per minute, and held there for ten minutes. The gas mixture consisted of 15% CO₂ and 85% N₂ by volume, flowing at a rate of 80 sccm. This initial heating in CO₂/N₂ ensured that the creation of a eutectic phase was achieved for each mixture, as will be discussed later. After ten minutes, the gas was switched to air for 20 minutes. The sorbent was cooled at a rate of 15 °C per minute to 550 °C. At 550 °C the CO₂/N₂ mixture was turned back on, and the sample was held isothermal for 30 minutes. At this point, the air replaced the CO₂/N₂ mixture and the sample was heated back to 800 °C at a rate of 10 °C per minute where it was held for 30 minutes. At

	Initial Ramp to 800 °C	Ramp to 550 °C	Isothermal 550 °C	Ramp to 800 °C	Cool to Room Temp
pure Li ₂ ZrO ₃	air	N ₂	CO ₂ /N ₂	N ₂	N ₂
Li ₂ ZrO ₃ w/calcined K ₂ CO ₃	N/A	N ₂	CO ₂ /N ₂	N ₂	N ₂
Li ₂ ZrO ₃ w/mixed K ₂ CO ₃	N/A	N ₂	CO ₂ /N ₂	CO ₂ /N ₂	N ₂
Li ₂ ZrO ₃ w/mixed Na ₂ CO ₃	CO ₂ /N ₂	CO ₂ /N ₂	CO ₂ /N ₂	CO ₂ /N ₂	CO ₂ /N ₂

Table 1. Gas flows used during each segment during the initial sorbent sample testing. n/a: Not available

	Description	Gas Mixture	Ramp rate (°C/min)	Final Temp (°C)	Time (min)
1	sorbent heated	CO ₂ /N ₂	15	800	N/A
2	sorbent held at isothermal temp	CO ₂ /N ₂	N/A	800	10
3	sorbent held at isothermal temp	air	N/A	800	20
4*	sorbent cooled	air	15	550	N/A
5*	sorbent held at isothermal temp	CO ₂ /N ₂	N/A	550	30
6*	sorbent heated	air	10	800	N/A
7*	sorbent held at isothermal temp	air	N/A	800	30
8*	sorbent cooled	air	10	550	N/A
9	sorbent cooled	air	10	room temp	N/A

Table 2. Method segments for testing the optimization samples. n/a: Not available *Segment repeated 3 times

the end of 30 minutes the sample was cooled to 550 °C at a rate of 10 °C per minute. This cycle was repeated three times (not including the initial heating to 800 °C in the CO₂/N₂ mixture). After the final period at 800 °C, the sample was cooled in air to room temperature.

Several experiments were run to test the stability of the sorbents during continuous CO₂ absorption and regeneration (Tables 3 and 4). The Li₂ZrO₃+Na₂CO₃ sample underwent multiple cycles of CO₂ absorption and desorption. The sorbent was heated in air at a rate of 10 °C per minute to a temperature of 700 °C, where

it was held in air for 60 minutes. It was then cooled at 10 °C per minute to 550 °C. At this point, the CO₂/N₂ gas mixture replaced air and the sorbent was held isothermally for one hour. The sample was then heated in air to 700 °C and was held there for 1.5 hours; after which time, it was cooled to 550 °C. This cycle was repeated fourteen times (excluding the initial temperature ramp), and after the final cycle, the sorbent was cooled to room temperature.

The method for testing sorbent regenerability was generally the same as the method for testing optimization (Table 2). All of the gas flows and holding times remained constant, however the

	Description	Gas Mixture	Ramp rate (°C/min)	Final Temp (°C)	Time (min)
1	sorbent heated	air	10	700	N/A
2	sorbent held at isothermal temp	air	N/A	700	60
3*	sorbent cooled	air	10	550	N/A
4*	sorbent held at isothermal temp	CO ₂ /N ₂	N/A	550	60
5*	sorbent heated	air	10	700	N/A
6*	sorbent held at isothermal temp	air	N/A	700	90
7*	sorbent cooled	air	10	550	N/A
8	sorbent cooled	air	10	room temp	N/A

Table 3. Method segments for testing Li₂ZrO₃+Na₂CO₃ regenerability. n/a: Not available *Segment repeated 14 times

	Description	Gas Mixture	Ramp Rate (°C/min)	Final Temp (°C)	Time (min)
1	sorbent heated	CO ₂ /N ₂	15	800	N/A
2	sorbent held at isothermal temp	CO ₂ /N ₂	N/A	800	30
3*	sorbent cooled	air	15	550	N/A
4*	sorbent held at isothermal temp	CO ₂ /N ₂	N/A	550	30
5*	sorbent heated	air	10	750	N/A
6*	sorbent held at isothermal temp	air	N/A	750	30
23**	sorbent cooled	air	10	550	N/A
24**	sorbent held at isothermal temp	CO ₂ /N ₂	N/A	550	30
25**	sorbent heated	air	10	800	N/A
26**	sorbent held at isothermal temp	air	N/A	800	30
27**	sorbent cooled	air	10	550	N/A
28	sorbent cooled	air	10	room temp	N/A

Table 4. Method segments for testing sorbent regenerability. n/a: Not available *Segment repeated at the respective regeneration temperatures: 760, 770, 780, 790 **Segment repeated 6 times

different regeneration temperatures were used and the number of cycles was increased to 11. After the initial heating to 800 °C, the regeneration temperatures were 750 °C, 760 °C, 770 °C, 780 °C, 790 °C and 800 °C respectively. The remainder of the experiment retained 800 °C as the regeneration temperature.

RESULTS AND DISCUSSION

Preliminary Samples

Figure 1a shows the CO₂ uptake curve for Li₂ZrO₃. The CO₂ uptake over the first 20 minutes of sorption is quite low, the rate being 7.08×10^{-3} mg CO₂/mg sorbent-h. These results are consistent with values reported by Pannocchia et al. In that study, it was shown that Li₂ZrO₃ had a low uptake rate, and the CO₂ uptake decreased significantly as time progressed [4].

Figure 1b shows the CO₂ uptake curve for the sorbent Li₂ZrO₃+K₂CO₃ sample made via method 1. The CO₂ uptake was 2.18×10^{-3} mg CO₂/mg sorbent-h. There is no definitive conclusion for why the uptake rate was lower for this sample, but it is known

from catalyst synthesis that the method of preparation can affect catalyst performance [5].

The CO₂ uptake curve for the sorbent sample of Li₂ZrO₃+K₂CO₃ that was prepared using method 2 is shown in Figure 1c. The CO₂ uptake rate for this sorbent is 7.24×10^{-2} mg CO₂/mg sorbent-h for the first 20 minutes of absorption. This rate is an order of magnitude larger than that of Li₂ZrO₃ and can be attributed to Li₂CO₃ and K₂CO₃ forming a eutectic liquid. These results can also be seen in other research [3].

Since a combination of Li₂CO₃ and K₂CO₃ increased the CO₂ absorption rate, it was decided that Na₂CO₃ should be tested as an additive to Li₂ZrO₃. This Li₂ZrO₃+Na₂CO₃ sorbent sample was prepared using method 2 as this was the method that had given better results with K₂CO₃. The uptake curve can be seen in Figure 1d. The CO₂ uptake rate was 1.70×10^{-1} mg CO₂/mg sorbent-h. This uptake rate was two orders of magnitude higher than that of the Li₂ZrO₃. For a comparison of the rates, see Figure 2.

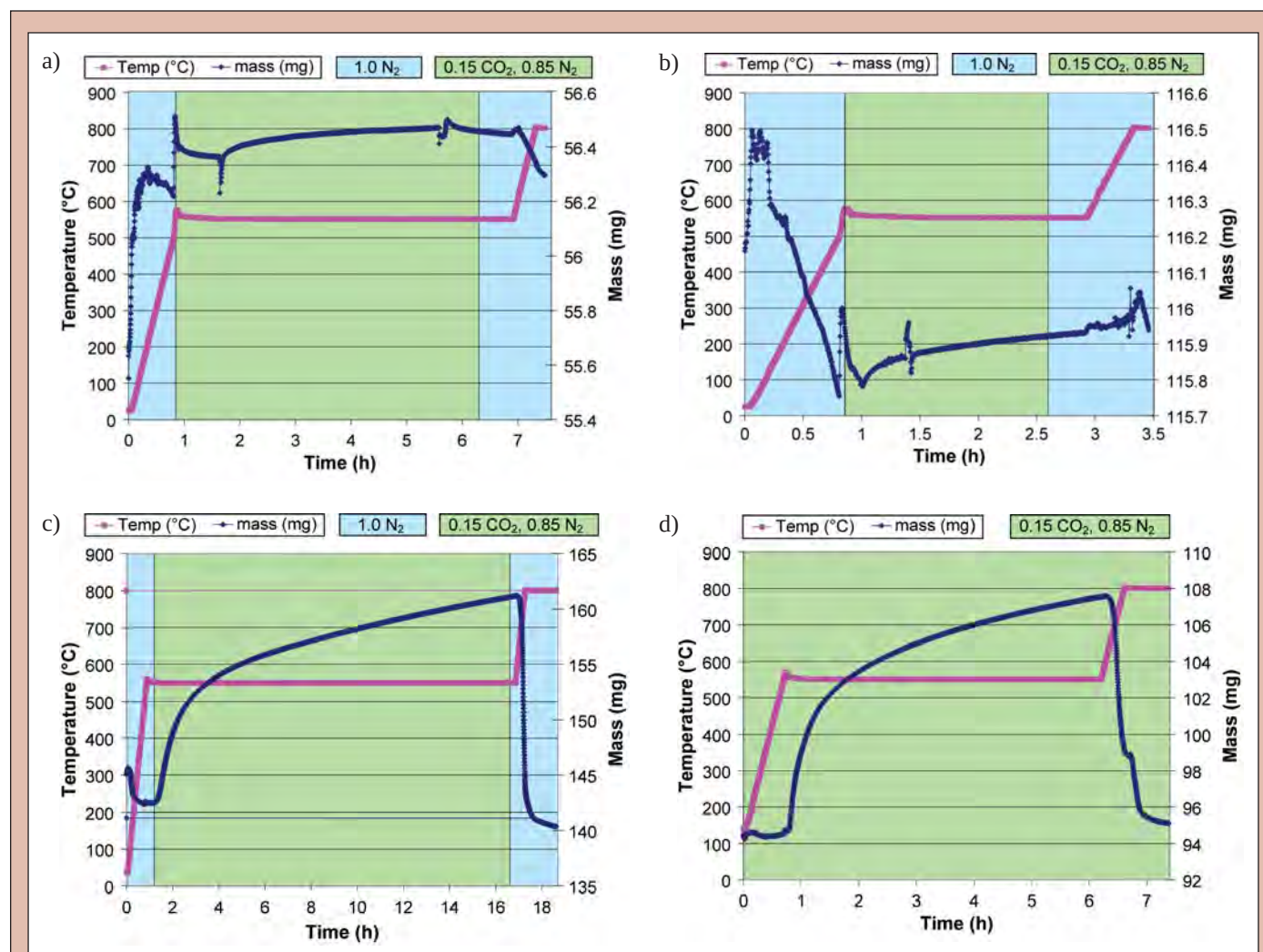
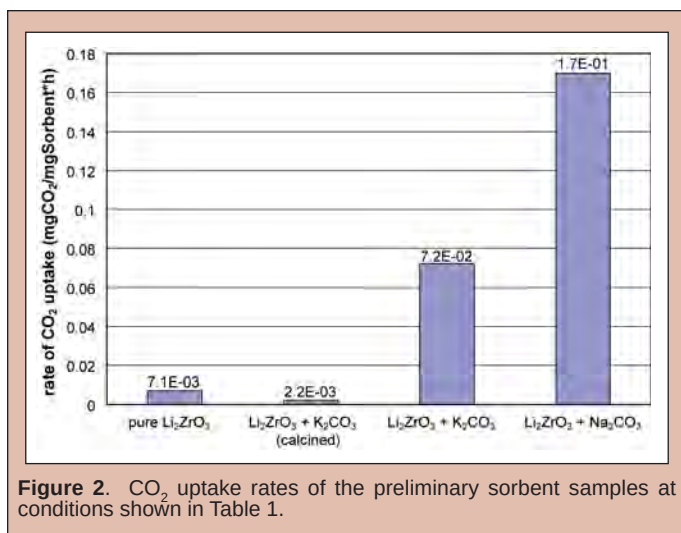


Figure 1. CO₂ uptake profiles from various Li₂ZrO₃ and additive combinations. Note that the gas compositions are given in fractions. a) Representative graph of mass and temperature versus time for CO₂ uptake for Li₂ZrO₃ without additives; b) representative graph of mass and temperature versus time for CO₂ uptake with Li₂ZrO₃ and K₂CO₃ mixture prepared by method 1; c) representative graph of mass and temperature versus time for CO₂ uptake with Li₂ZrO₃ and K₂CO₃ mixture prepared by method 2; d) representative graph of mass and temperature versus time for CO₂ uptake with Li₂ZrO₃ and Na₂CO₃ mixture prepared by method 2.



Optimization Experiments

The addition of both K₂CO₃ and Na₂CO₃ resulted in an increase in the uptake rate of CO₂. It was decided that experiments should be run to see if there is a ratio of K₂CO₃ to Na₂CO₃ that would give a maximum uptake rate. The foundation for each sorbent sample was 1 g of Li₂ZrO₃, and varying quantities of K₂CO₃ and Na₂CO₃ were added. The quantity of either additive was determined using a sequential simplex optimization method [6]. The optimization was based on the weights of each additive and the objective function was the average uptake rate over the first 20 minutes of absorption. The preliminary experiments showed that a small amount of either additive would increase the uptake rate of CO₂. To set a basis for the optimization experiment, two samples were made using either K₂CO₃ or Na₂CO₃ only, both of which were large quantities when compared to the preliminary samples. Sample 1, containing approximately 0.5 g of K₂CO₃, had a CO₂ uptake rate of 9.72×10^{-3} mg CO₂/mg sorbent·h. Sample 2, containing approximately 0.5 g of Na₂CO₃, had a CO₂ uptake rate of 2.17×10^{-2} mg CO₂/mg sorbent·h. A total of 17 mixtures were tested with results shown in Figure 3a. Sample 13, composed of 0.9998 g Li₂ZrO₃, 0.1887 g K₂CO₃ and 0.1742 g Na₂CO₃, gave the best results, with an uptake rate of 1.956×10^{-1} mg CO₂/mg sorbent·h. Unfortunately, the optimization study had to be terminated prematurely due to time constraints, so further testing needs to be done in order to determine if this is the best possible mixture.

Note that both samples 1 and 2 have lower uptake rates than the preliminary test samples containing lesser amount of K₂CO₃ or Na₂CO₃ added to Li₂ZrO₃, demonstrating that the quantity of each compound added to the Li₂ZrO₃ base has a direct affect on the uptake rate. Figure 3b shows weight fractions of each additive contained in the optimization samples and the respective rates of CO₂ uptake.

A significant loss of mass from the sorbent was seen during some of the tests. During the regeneration cycles, the sorbent lost more mass than it gained during the absorption of CO₂; this can be seen in Figure 4. Pannocchia et al. hypothesized that at high temperatures, potassium in the sorbent is oxidized while in air and is released from the sample [4]. Regeneration in N₂ showed no weight loss at 800 °C.

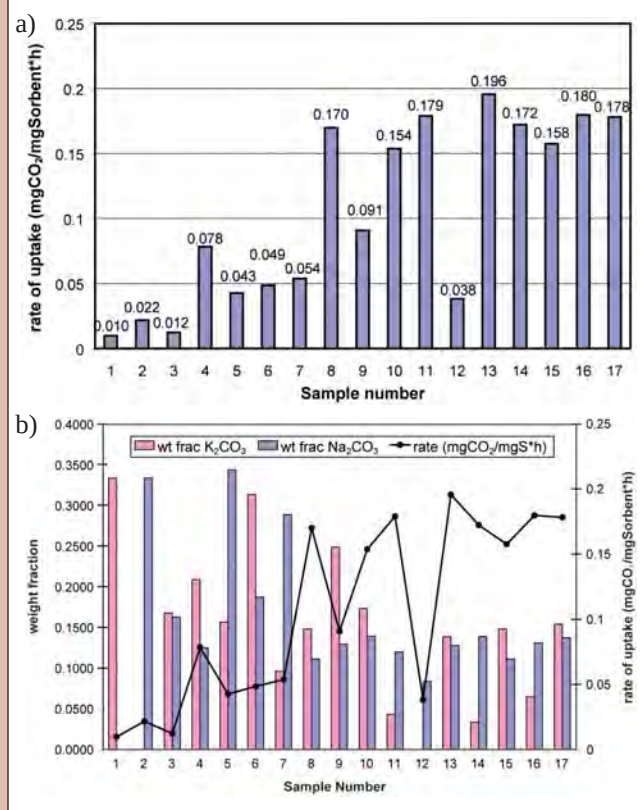
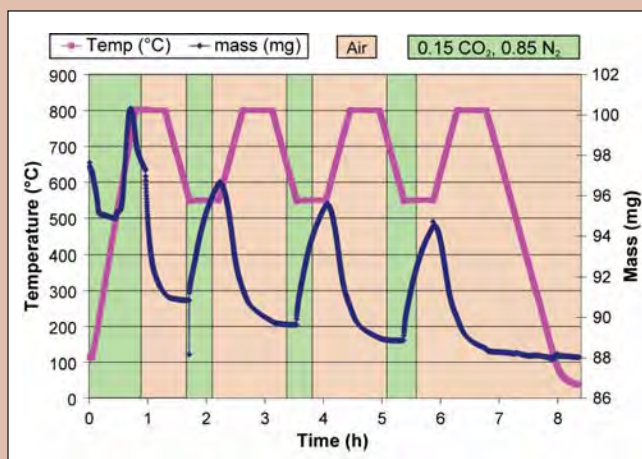


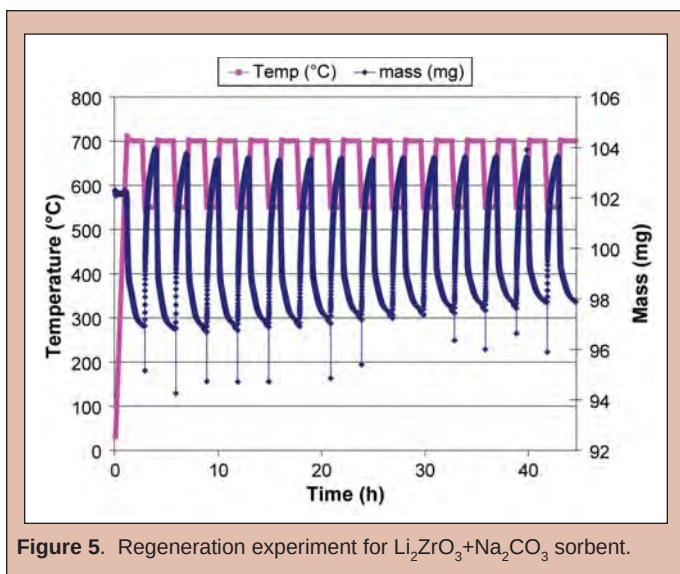
Figure 3. a) CO₂ uptake rates for the optimization samples; b) weight fractions of K₂CO₃ and Na₂CO₃ and the respective CO₂ uptake rates.



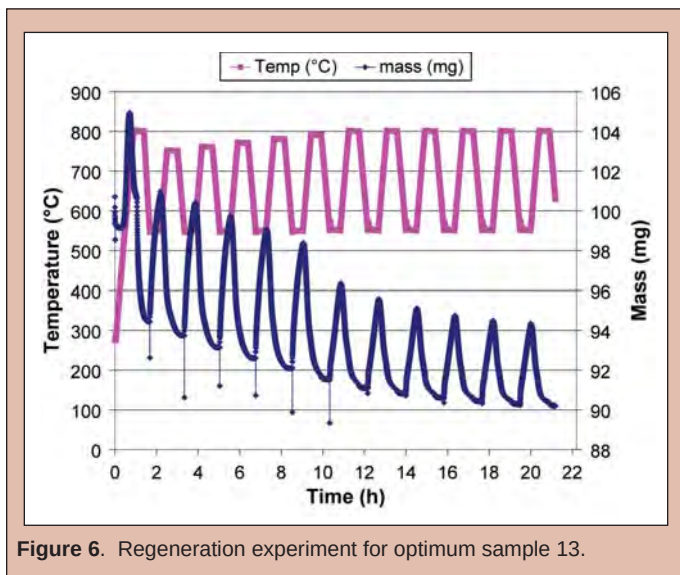
Regeneration Experiments

The preliminary sample containing Na₂CO₃ and sample 13 from the optimization samples were tested for CO₂ uptake stability.

Over the course of 14 cycles, the Li₂ZrO₃+Na₂CO₃ sample showed steady CO₂ uptake and release. The uptake rate for the first cycle was 1.37×10^{-1} mg CO₂/mg sorbent·h, and the uptake rate for the final cycle was 1.93×10^{-1} mg CO₂/mg sorbent·h. The final rate was 40% higher than that of the initial cycle. Since the absorption rate increased over time, the sample can be considered stable. See Figure 5 for the regeneration experiment results.



As noted before, certain sorbents from the optimization samples lost significant amounts of mass while regenerating. A regeneration test was conducted on sample 13 from the optimization sample set. This test operated at various regeneration temperatures to determine if mass loss occurred at temperatures lower than 800 °C, and whether or not the uptake capacity remained constant. The sorbent lost noticeable amounts of mass despite the lower regeneration temperatures. Throughout the experiment, the absorption rate decreased, and at cycle 6 the absorption rate was significantly reduced. The absorption rate decreased for the remainder of the experiment. The initial uptake rate was 1.57×10^{-1} mg CO₂/mg sorbent-h; the rate at cycle 6 was 1.07×10^{-1} mg CO₂/mg sorbent-h; the final absorption rate was 9.43×10^{-2} mg CO₂/mg sorbent-h. The fluctuations of both the mass and absorption rates deem the sorbent to be unstable as shown in Figure 6. Although it appears to be temperature dependent, the reason for the steady drop in the mass and corresponding absorption rates has not been determined and will be the subject of a future study.



CONCLUSION

The objective of this study was to determine the CO₂ absorption rate of various Li₂ZrO₃-based sorbents. Li₂ZrO₃ has an infinite CO₂/N₂ selectivity, and has the ability to regenerate at relatively low temperatures, making it an excellent sorbent for CO₂ capture from complex gas streams. Li₂ZrO₃ had essentially a zero CO₂ uptake rate, but with the addition of K₂CO₃ and Na₂CO₃, the uptake rate increased significantly. It was also found that a mixture of both K₂CO₃ and Na₂CO₃ with Li₂ZrO₃ results in a larger uptake rate than either sorbent prepared with only one of the additives. Additionally, regenerability tests performed on one sorbent gave favorable results, allowing it to be considered stable. Sample 13 from the optimization study showed extensive mass loss when tested at high regeneration temperatures. Tests done at lower regeneration temperatures showed that significant mass loss still occurred at temperatures higher than 700 °C, but when regenerating at or below 700 °C, the sorbent stability remained constant. Future testing may resolve the mass and absorption rate decreases.

Testing of the Li₂ZrO₃ sorbent under real syngas conditions should be done in the future. These experiments would include testing the sorbent with gases comparable in composition with syngas, as well as introducing the sorbent to higher pressure. Once an optimum sorbent has been found, a support system that would be suitable for an actual reactor will be needed.

ACKNOWLEDGEMENTS

I would like to thank Yves Parent for providing me with the necessary testing equipment and for sharing his extensive knowledge on sorbents, and also Matthew Yung and Whitney Jablonski for assisting me in many minor tasks around the laboratory. Furthermore, I would like to give special thanks to Linda Lung and the NREL Office of Education for hosting the SULI program, as well as the Department of Energy, Office of Science for making this internship possible.

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DEVELOPMENT OF ACCELERATOR DATA REPORTING SYSTEM AND ITS APPLICATION TO TREND ANALYSIS OF BEAM CURRENT DATA

MARIANO J. PADILLA AND WILLEM BLOKLAND

ABSTRACT

Detailed ongoing information about the ion beam quality is crucial to the successful operation of the Spallation Neutron Source at Oak Ridge National Laboratory. In order to provide the highest possible neutron production time, ion beam quality is monitored to isolate possible problems or performance-related issues throughout the accelerator and accumulator ring. For example, beam current monitor (BCM) data is used to determine the quality of the beam transport through the accelerator. In this study, a reporting system infrastructure was implemented and used to generate a trend analysis report of the BCM data. The BCM data was analyzed to facilitate the identification of monitor calibration issues, beam trends, beam abnormalities, beam deviations and overall beam quality. A comparison between transformed BCM report data and accelerator log entries shows promising results which represent correlations between the data and changes made within the accelerator. The BCM analysis report is one of many reports within a system that assist in providing overall beam quality information to facilitate successful beam operation. In future reports, additional data manipulation functions and analysis can be implemented and applied. Built-in and user-defined analytic functions are available throughout the reporting system and can be reused with new data.

INTRODUCTION

The Spallation Neutron Source (SNS) is a pulsed neutron source that uses the most power in the world for use in scientific research and industrial development. In order to achieve the production of neutrons at the target using 1.4 megawatts (MW) of operating power, the SNS Beam Instrumentation Group (BIG) monitors the accelerator performance. Proper beam quality and transport will ensure high availability of neutrons for user experiments. To facilitate the monitoring of the accelerator at multiple levels, from the control room to executive summary reports, a reporting system was first envisioned in a LabVIEW display [1], [2]. A prototype was developed by Madhan Sundaram, Neutron Science Systems Software Engineer at Oak Ridge National Laboratory (ORNL) using MySQL, Personal Home Page (PHP), Asynchronous JavaScript and Extensive Markup Language (AJAX) scripting. The prototype demonstrated the ability to refine the initial reporting capability of a database using

a common web interface for viewing. The prototype was developed further during the summer of 2007 to incorporate Java programming for data acquisition and to interface with an Oracle database cluster recently introduced at SNS. The reporting system continued to be developed at ORNL by Jeff Patton, Software Systems Administrator, and Douglas J. Edwardson, Scientific Systems Programmer, both within the Oracle database and with the modification of the user interface to use Adobe's Flex Technology. The revamped reporting system accesses data stored in the database and implements Java classes incorporating pre-defined and user-defined analytic functions. The reporting system will be the foundation for analyzing data taken throughout the accelerator. It provides a simple and intuitive user interface that is cross-platform and easily accessible for the design, viewing and distribution of reports throughout SNS or outside the SNS facilities (via e-mail).

METHODS

The reporting system consists of five processes or methods, also shown in Figure 1. Each process is defined here. 1) *Report Definition* is the interface where the user defines the data to be acquired, how to process the data into the desired results and how to format and publish the results, 2) *Data Collection* is the process that takes the data from the accelerator, 3) *Database Storage* is the process of storing data within an optimized data storage system to facilitate retrieval and processing of data, 4) *Report Processing and Logic* is the process that takes the data stored in the Oracle database and transforms it into the results that will be used in the report and 5) *Report Delivery* is the process that formats the processed data into a report (pdf, image, flex) and delivers as defined (email, database or web server).

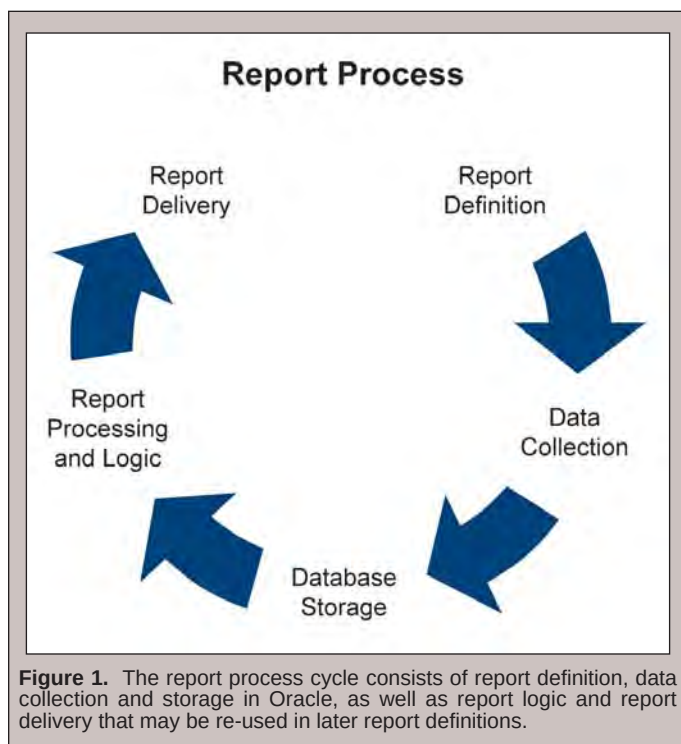


Figure 1. The report process cycle consists of report definition, data collection and storage in Oracle, as well as report logic and report delivery that may be re-used in later report definitions.

The report definitions, the processing functions, or the report formatting can be reused to create another report. The database stores the report definition, the raw data, the results and the final report. The database also links the processes together and is thus central to the reporting system. Figure 2 shows how these five processes have been implemented. The next sections explain in further detail the function of the five processes.

Report Definition

The report definition includes graphical report display choices, published data from the accelerator in the form of a list of process variables (PVs), and a selection of Oracle Structured Query Language (SQL) code. The report logic is also defined in this section and consists of basic pre-defined Java classes, such as simple scalar addition, multiplication or division, and specialized user-defined Java classes. Each report definition is saved in the database and can be used as a template for future reports. Users will be able to select previously defined reports, to modify or re-use in their own report.

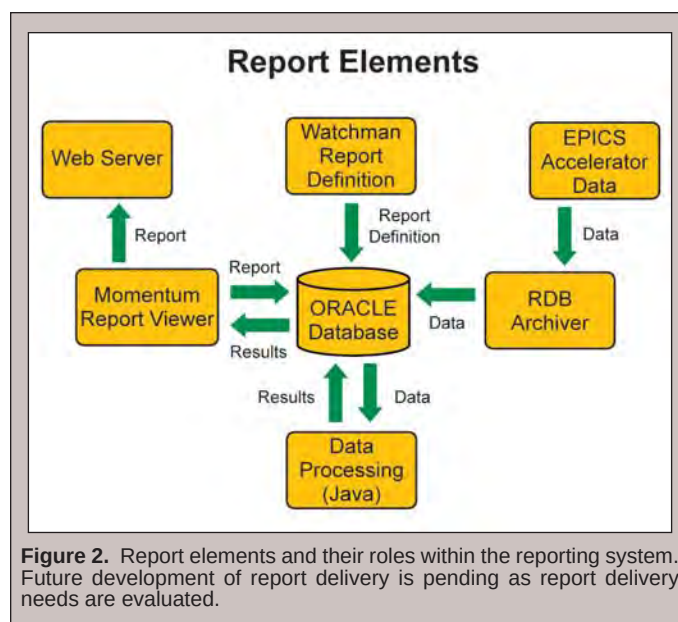


Figure 2. Report elements and their roles within the reporting system. Future development of report delivery is pending as report delivery needs are evaluated.

Data Collection

Data collected from the accelerator is archived within the Oracle database and used by the reporting system. The data storage uses Oracle record definitions which are already present, both for archiving and reporting, so that an existing data collection mechanism can be used. Also, as data is archived, future reports can recall historical data, thus extending the flexibility of the reporting system. Manipulated or analyzed data is also stored in the Oracle database, allowing future reports to re-use analyzed data.

Database Storage

At the center of the system is the Oracle database. The reporting system takes advantage of the power of the database cluster and is projected to grow along with the archiving needs. Oracle also provides pre-built analytic functions, such as average and standard deviation. In addition to performance, using Oracle as a central storage for all data, raw and processed, allows reports to re-use existing data without duplication. Although SNS chose Oracle because of its availability, the reporting system does not depend on Oracle and can be used with other databases.

Report Processing and Logic

The reusable report logic contains Oracle SQL statements for standard deviation, average, and other statistics reporting functions. It also includes user-defined Java programming language classes that can be chained for execution within a report to further manipulate data. The Oracle SQL statements are stored in the database, while the user-defined Java classes are stored as Java class files. Users can create new logic even when they are not producing reports. The Java logic is stored and made available for any report definition. Upon selection of the Java logic, the report engine will execute the logic for processing the data.

Report Delivery

The report delivery publishes the results defined in the delivery options such as PDF, PNG export, and/or e-mail delivery of the PDF or PNG files. All reports can be viewed through the web

Reporting System Elements

Report Definition: The Watchman report definition element is a web interface where the authenticated user defines the PVs, date range and data summarization for the report. The interface is an intuitive flash web page designed using Flex. Flex implements Adobe's Flash technology to incorporate a simple, efficient, and elegant interface design. Figure 3 shows the data section of the Watchman user interface, where users select the PVs for their report. Figure 4 shows the chart section of the Watchman user interface, where the users define chart options such as line graph, line color,



Figure 3. Watchman user interface. PVs/IOCs selection screen.



Figure 4. Watchman Chart definition user interface.

Figure 5. Watchman Report metadata definition user interface.

Database Storage: The database uses multiple table definitions and data field definitions within the database known as schemas. Depending on summarized data or raw data needed for the report, the data is stored within the appropriate schema in the Oracle database. The reporting system accesses the raw data from the channel archive schema and makes it available to the data and diagnostics reporting system schema for producing pre-defined reports. Within the data and diagnostics report system schema,

processed or summarized data can be stored for reuse in future reports. Oracle executes statistical functions at the cluster level, making Oracle not only a central storage element of the reporting system, but also a processing element.

Report Processing and Logic: The report engine consists of several Java classes that query data from the Oracle database, execute user-defined Java classes, and implement distribution options. The report engine can call the Momentum viewer to display the chart, or can generate PDF or PNG graphic exports to be e-mailed or stored in the file system. The report engine tier of the reporting system runs on a production web server and is written entirely in Java programming language. It runs continuously and produces reports by launching independently running processes (program threads) which execute report-generating Java programming classes defined by the user.

These Java programming language classes defined by the user are integrated into the report engine. Figure 6 shows a sample user-defined Java class that generates the beam current monitor (BCM) trend analysis report. Other user-defined Java classes can be implemented to create additional customized reports which may then be reused in other reports or chained as part of a list of processing steps to achieve desired data manipulation within the reports.

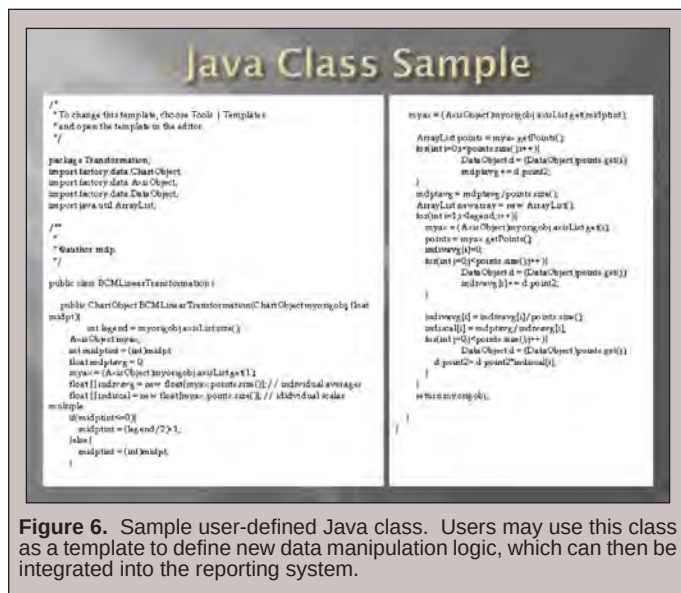


Figure 6. Sample user-defined Java class. Users may use this class as a template to define new data manipulation logic, which can then be integrated into the reporting system.

Report Delivery: The Momentum web page is a common Flex-based web page where users can view their reports and charts. In the current version of the Momentum viewer, charts are displayed based only on the defined report logic. The analytic functions and Java logic have already been implemented by the report engine prior to charting the data. All data already processed, as per the user's instructions, is then delivered to the Momentum viewer as a chart. The viewer has the option to export to PDF.

BCM Trend Analysis Report

One of the reporting templates, a BCM Trend Analysis report, is designed by graphing raw data collected at 1 Hz intervals and averaged every 60 records. The data collected is the charge of the particle beam as measured by the various BCMs at given times. The data is averaged as denoted as sequence $\{y_t\}_{t=1}^N$, representing

a moving average sequence [6]. Given a sequence $\{y_t\}_{t=1}^N$, with y_t being the charge measured at time t , an n -moving average is a new sequence $S_n = \{s_t\}_{t=1}^{N-n+1}$ defined from the y_t by taking the average of subsequences of n terms.

$$s_t = \frac{1}{n} \sum_{j=t}^{t+n-1} y_j \quad (1)$$

Figure 7 shows the decimated average charge for several BCMs as functions of time or multiple sequences S_n^k with k the index identifying a BCM. Any trends in this graph are hard to see because the signals vary widely from one BCM to another. Recalibration of the data is necessary to clearly see the trends.

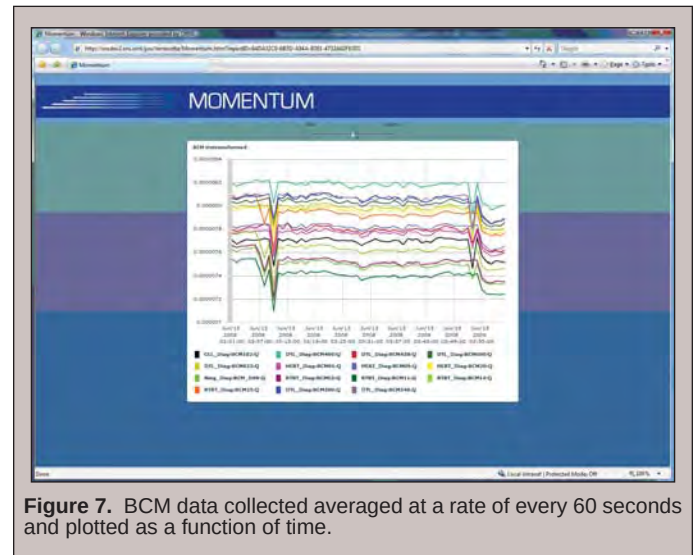


Figure 7. BCM data collected averaged at a rate of every 60 seconds and plotted as a function of time.

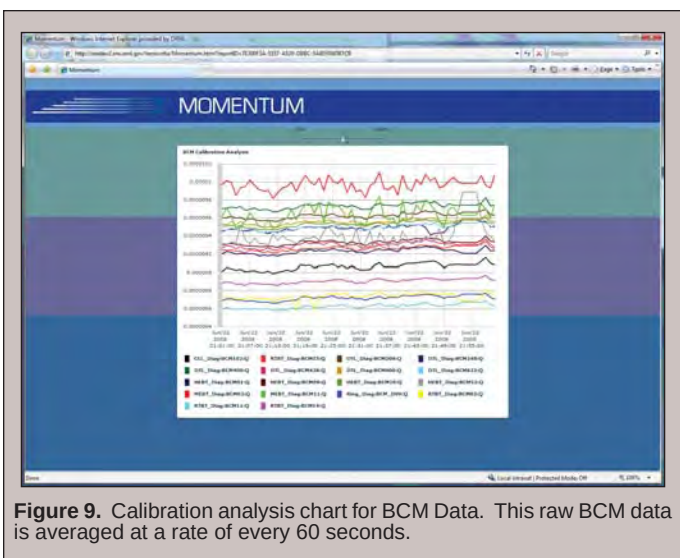
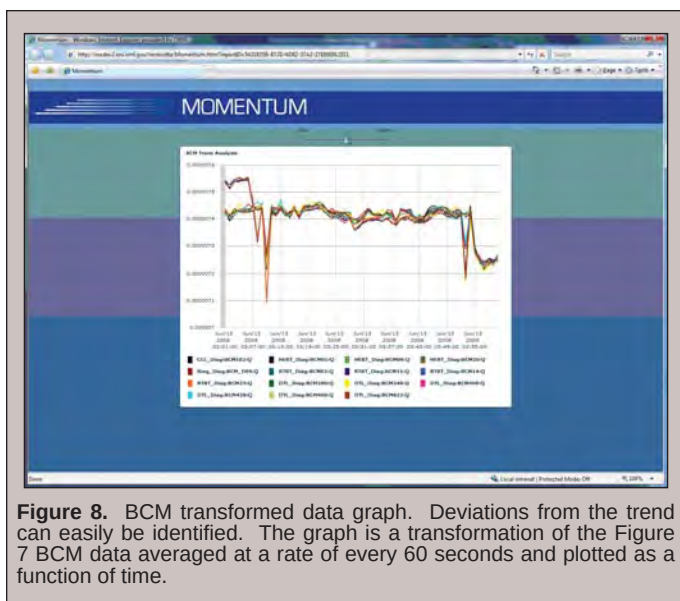
The BCMs sequences S_n^k are calibrated by taking the average of the sequence from one pre-selected BCM and multiplying each sequence from the other BCMs with this reference average divided by the average of each BCM sequence. These averages are not taken over the whole sequence but just over that part of the sequence where the beam was stable and no modifications were made to the accelerator. The results are new sequences S_n^{*k} with k the BCM index and R_k the scaling factor for BCM k

$$S_n^{*k} = R_k S_n^k \quad (2)$$

where K denotes a pre-selected sequence used as a baseline, $i = 1$, the first sequence sample and M the number of sequence samples used for the averaging

$$R^k = \frac{1}{M} \sum \{S_i^K\}_{i=1}^{M-n+1} / \frac{1}{M} \sum \{s_i^k\}_{i=1}^{M-n+1} \quad (3)$$

A decimation of sequences S_n^{*k} is graphed as shown in Figure 8. In contrast to sequences S_n^k that are shown in Figure 7, the trends and variations are easily spotted in Figure 8.



RESULTS

The reports designed thus far have obtained good results that can be correlated to events within the accelerator operations and to configuration changes of instrumentation. Since the reporting system is designed to encompass more than one aspect of reporting for the entire accelerator, three different results are presented here.

Noise

In the chart in Figure 9, the BCMs in the Medium-Energy Beam Transport (MEBT) and High-Energy Beam Transport (HEBT) sections of SNS, MEBT_Diag:BCM02:Q, MEBT_DiagBCM11:Q and HEBT_Diag:BCM32:Q show more noise and larger standard deviation than the rest of the BCMs. The greater standard deviation in the report for the MEBT BCM is probably due to low frequency noise affecting the charge calculation. A different grounding scheme is being investigated to alleviate this problem. The noisy signal in HEBT BCM32 occurs because of its close proximity to the Ring devices. Because of the known grounding and noise issues, BCM02 and BCM11 from the MEBT section of the accelerator and BCM32 from the HEBT section are excluded from the BCM Trend Analysis Report. Thus, grounding and noise issues are easily identified in the report.

Event Correlation

In the data shown in Figure 8, which was collected on June 13, 2008, the transformed BCM Trend Analysis report shows a change in the trend from 3:00 AM to 3:06 AM. The change, as later reported in the Accelerator Electronic Logs (E-log), correlates with an entry explaining the movement of stripping foil position near the I-dump section of the accelerator. Ring_Diag:BCM_D09:Q, RTBT_Diag:BCM02, RTBT_Diag:BCM11:Q, RTBT_Diag:BCM14:Q and RTBT_Diag:BCM25:Q display a difference of approximately 1.0×10^{-7} during the period of June 13, 3:00 AM to June 13, 4:00 AM.

Systematic Error

In a theoretical model for calibration of BCMs, all graphs should lie within a standard deviation of 1.0×10^{-7} , however, the current graphs have a deviation of approximately 8.0×10^{-7} . This report indicates possible imperfections in the monitors. The results also indicate that the BCM calibration can be improved.

DISCUSSION AND CONCLUSION

The reporting system is the result of a collaboration of technology and individuals. The technologies meld together as the integration of the report extends from EPICS to Oracle and out to the user via a web interface. The integration of ongoing development, such as the RDB Data Archive and Oracle, makes the reporting system possible and will provide further feedback for data archiving needs. For example, as reports are generated and used over a period of time, trends within the reports will provide guidance on these needs. If the reports require only summarized data, then the data acquisition can be further customized to collect at the adjusted interval, or the data can be summarized for long-term archiving.

The purpose of the RDB Data Archive is to archive all data from the accelerator for all defined PVs. The reporting system makes use of this technology, rather than developing a new one, in order to assist the developer in providing feedback and in refining the development of the RDB Data Archive, as well as integrating existing and new technology to be part of the overall reporting system. Though the RDB Data Archive has milestones and goals outside the reporting system, the integration of the technology was the best fit for the reporting system.

The Java logic implementation allows users to specify specific logic for data manipulation. Additional signal filtering routines can be implemented to extend the analysis of the reporting system. The ability to extend the reporting system's analysis tools by writing Java classes gives the reporting system a flexibility and reusability that will grow. An example is the BCM Analysis Report.

As is the case with much software, the results presented here show that the BCM Analysis Report needs to be enhanced. The analysis for Figures 7 and 8 shows a higher overall charge during the time period of 3:00 AM to 3:06 AM. The results of the data

transformation should have reflected this fact. The transformation applied uses the average of the entire series, thus when the Ring and RTBT BCMs were adjusted, the adjustment should be calculated over the period of 3:00 AM to 3:06 AM to get the proper average adjustment. The variation in the report coincides with operator adjustment of the stripping foil in the ring section of the accelerator; therefore a lower overall average charge should be represented after the adjustment. The BCM Transformation Report succeeded in representing an abnormality within the operations of the accelerator; however, an additional parameter in the algorithm is needed to represent data more accurately. The additional parameter needed is to better define the multiplicative factor used in the transformation. Currently it is a ratio of the averages between the reference series and the series to be transformed. The reference series average is taken over the entire dataset and thus reflects an overall average, rather than the section where the discrepancy occurred. Although the transformed chart reported good results for the trend analysis, the additional parameters will allow for the definition of the timeframe for the ratio. Instead of calculating averages over the entire timeframe of the chart, the user will be able to define the averages for only a section of the series' timeframe. This additional parameter will allow the report to better reflect the true value of the factor to be applied to the calibrations between BCMs. The true value takes into consideration the beam loss changes.

The reporting system is currently used only with BCM data; however, future implementation will include neutron detector data to generate a Contact Radiation Decay Report and Beam Loss Monitor (BLM) data to provide summaries of total beam loss throughout the accelerator.

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PRELIMINARY IN-SITU X-RAY ABSORPTION FINE STRUCTURE EXAMINATION OF Pt/C AND PtCo/C CATHODE CATALYSTS IN AN OPERATIONAL POLYMER ELECTROLYTE FUEL CELL

BRIAN T. PHELAN, DEBORAH J. MYERS AND MATT C. SMITH

ABSTRACT

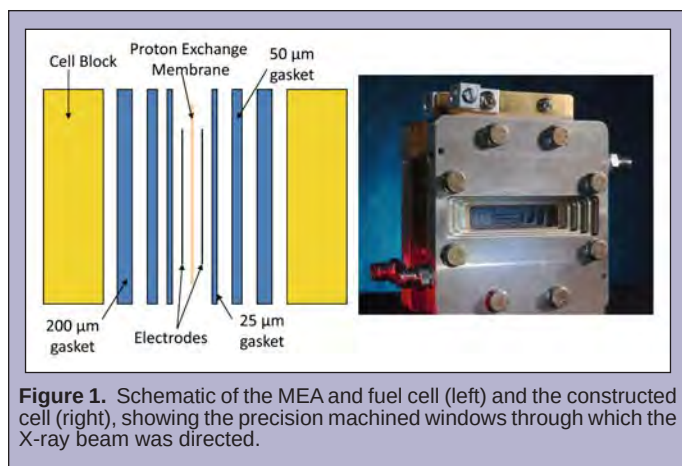
State-of-the-art polymer electrolyte fuel cells require a conditioning period to reach optimized cell performance. There is insufficient understanding about the behavior of catalysts during this period, especially with regard to the changing environment of the cathode electrocatalyst, which is typically Pt nanoparticles supported on high surface area Vulcan XC-72 carbon (Pt/C). The purpose of this research was to record preliminary observations of the changing environment during the conditioning phase using X-Ray Absorption Fine Structure (XAFS) spectroscopy. XAFS was recorded for a Pt/C cathode at the Pt L₃-edge and a PtCo/C cathode at both the Pt L₃-edge and Co K-edge. Using precision machined graphite cell-blocks, both transmission and fluorescence data were recorded at Sector 12-BM-B of Argonne National Laboratory's Advanced Photon Source. The fluorescence and transmission edge steps allow for a working description of the changing electrocatalyst environment, especially water concentration, at the anode and cathode as functions of operating parameters. These features are discussed in the context of how future analysis may correlate with potential, current and changing apparent thickness of the membrane electrode assembly through loss of catalyst materials (anode, cathode, carbon support). Such direct knowledge of the effect of the conditioning protocol on the electrocatalyst may lead to better catalyst design. In turn, this may lead to minimizing, or even eliminating, the conditioning period.

INTRODUCTION

Polymer electrolyte fuel cells (PEFCs) are approaching commercial viability as an efficient alternative to the internal combustion engine (ICE). Hydrogen-fueled PEFCs are targeted for automotive applications due to their high efficiency and benign emissions [1]. PEFCs are currently used for stationary applications due to the less demanding conditions, such as a relatively constant load and well-controlled environment. The load in automotive applications is constantly changing, exacerbating catalyst degradation through mechanisms associated with repeated oxidation and reduction of the catalyst, and is a major issue preventing widespread fuel cell adoption [2]. Additional issues include the cost of platinum

group metal (PGM) electrocatalysts (such as Pt or Pd) used in fuel cells and the conditioning phase required to reach optimal performance.

The PEFCs studied in this investigation are constructed with a proton exchange membrane (PEM) separating the anode and cathode catalysts, which in turn are sandwiched between gas diffusion layers, compression gaskets and graphite cell blocks (Figure 1). Cutting-edge electrocatalysts are nanoparticles supported on carbon which maximize the surface area of the electrocatalyst and minimize precious metal loadings, thus minimizing cost. A second technique employed to minimize the use of precious metal and



increase durability and activity is doping the PGM with a common base metal, such as cobalt, iron or nickel [3].

State-of-the-art Pt-containing cathode electrocatalysts benefit from a conditioning phase prior to sustained operation to attain improved and stabilized performance [4]. Different protocols exist for implementing the conditioning phase. These protocols include: changes in runtime, electrical conditions, humidity levels and temperatures of the fuel cell and gases [4]. There is insufficient understanding of the conditioning phase, though it is widely accepted that the processes responsible for conditioning are either modifications of catalyst structure, humidifications of the ionomer in the electrode layer or of the membrane, or the establishing of three-phase boundaries in the electrocatalyst layers. Increased knowledge of the changes in the catalyst layers (primarily for the cathode electrocatalyst since oxygen reduction at the cathode is the kinetically limiting event in the fuel cell reaction) and of the dynamic environment within the fuel cell will improve future catalyst design and refine operational parameters, cell configuration and assembly. Ultimately this may yield designs that can minimize, or even eliminate, the time and material costs of conditioning.

X-ray Absorption Fine Structure (XAFS) spectroscopy is an ideal tool for probing PEFCs in-situ since X-ray radiation can be tuned to the energy of electronic interactions in specific atomic species [5]. In-situ spectroscopy, as opposed to traditional post mortem style ex-situ analysis, permits observation of the catalyst during the conditioning phase, allowing interpretation of changes as they occur.

Here, the focus was on Pt-based cathode electrocatalysts, including a Pt on C (Pt/C) electrocatalyst and a PtCo alloy on C (PtCo/C) electrocatalyst. XAFS was recorded at the Pt- L_3 edge for the Pt/C cathode and at the Pt- L_3 edge and Co-K edge, separately, for the PtCo/C cathode. When energies are tuned at or above the absorption edges for Pt and Co respectively, incident X-rays are absorbed by the Pt and Co atoms in the X-ray beam path. This results in excitation of an electron within the atoms and a corresponding decrease in the transmission of X-rays through the entire sample. The decrease in transmission is thus correlated with absorption of X-rays at both the anode and cathode. When the X-rays are of sufficient energy to eject electrons from a core shell of the absorbing atom, a vacancy is created which is filled by an electron from an outer shell, producing fluorescence. The fluorescence wave does not traverse through the entire cell. It only interacts with materials from the cathode and thus contains information solely

pertaining to the cathode. XAFS data is manipulated mathematically to provide information of the atomic environment, typically yielding information on coordination and oxidation states of the absorbing atom and of neighboring atoms, and bond distances.

The XAFS spectra can be broken down into three portions, the pre-edge, the absorption edge (X-ray Absorption Near Edge Structure, XANES) and the post-edge (Extended X-ray Absorption Fine Structure, EXAFS). The focus of this paper is a preliminary qualitative analysis involved with the variations observed in the edge step, $\Delta\mu(E_0)$, which is the difference in height at the absorption energy, E_0 , between an algorithm fitted to the pre-edge and an algorithm fitted to the post-edge (Figure 2) [6]. Correlations and disparities between the changes in edge steps between scans provide information relevant to the environment within the PEFC, especially regarding water volume at the electrodes and the quantity of mass present within the beam. A detailed directory of the possible changes in edge steps along with credible explanations for each situation can be found in Table 1. Two Pt-Pd membrane electrode assemblies (MEAs) with Pt/C and Pd/C cathode and anode electrocatalysts respectively, and two PtCo/C cathode and Pd/C anode MEAs were conditioned through stage 1 and stage 2 of a protocol recommended for cell conditioning by the United States Fuel Cell Council (USFCC) [4]. Transmission and fluorescence was recorded for each MEA throughout the conditioning phase, however several scans had to be discarded because of glitches in the spectra, large drops in signal typically due to water bubbles passing through the cell. The edge steps of the fluorescence and transmission spectra were analyzed and employed to explain the catalyst condition and cell environment during the conditioning phase.

	Fluorescence Edge Step	Transmission Edge Step
Increase	Loss of H ₂ O on cathode	Gain of H ₂ O
Decrease	Gain of H ₂ O, loss of Pt	Loss of H ₂ O, carbon support, Pt, or Pd

Table 1. Correlation of an increase or a decrease in the fluorescence or transmission edge step with fuel cell events.

METHODS

Theoretical

XAFS spectra were recorded simultaneously in transmission and fluorescence geometries. The focus of this analysis is the edge step of the spectra, a value obtained by fitting one algorithm to the pre-edge and a second algorithm to the post-edge, extending both algorithms beyond the absorption edge and calculating the difference between the two lines (algorithms) (Figure 2).

The XAFS equation is given as:

$$\frac{I_0}{I_1} = e^{-\mu x} \quad (1)$$

where μ is the absorption coefficient of the absorbing species and x is the thickness of the material within the beamline. For the transmission spectra, I_0 represents the beam energy before encountering the cell and I_1 represents the transmission recorded. The fluorescence spectra were qualitatively analyzed under the simplified assumption that the ratio of the fluorescence detected to the original beam was proportional to the right hand side of Equation 1. The results will be represented in terms of apparent thickness, as the absorption coefficient of the absorbing species is

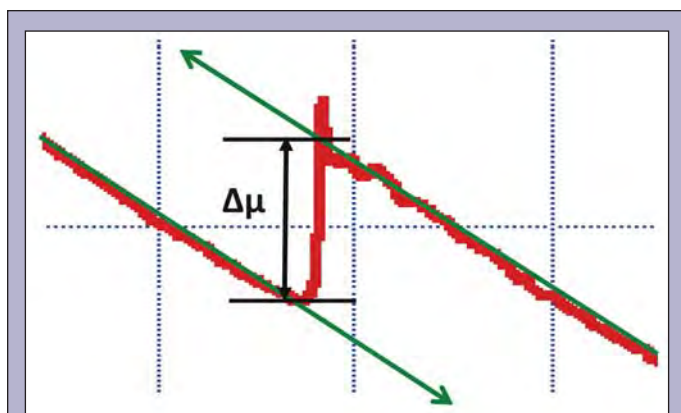


Figure 2. Edge step of a transmission spectrum. The edge step is the difference between the algorithm fitted to the pre-edge and post-edge at the absorption energy. This description can be applied to fluorescence spectra as well.

constant. This leaves any change in edge step to be caused by x , the thickness of the material within the path of the beam.

Changes in the edge step can be interpreted as meaningful observations regarding the dynamic state of the fuel cell. Fluorescence events will only portray information pertaining to the cathode as the fluorescence has a limited penetration depth. Transmission data can yield information on either the cathode or anode, allowing for the detection of differences between the events and environments on both the anode and cathode.

Experimental

XAFS spectra were recorded at Sector 12-BM-B, a bending magnet beamline, at the Advanced Photon Source at Argonne National Laboratory (ANL) using a Si(111) monochromator detuned at least 10% to reject higher harmonics. Data were acquired in transmission and fluorescence geometries using an ionization chamber, ionization chamber 1 and a liquid dinitrogen cooled 13-element Ge detector respectively. Measurements were obtained using precision machined graphite cell blocks that had windows milled down to 12 one thousandths of an inch on each side, allowing for transmission data collection. Spectra were analyzed using standard methods with the ATHENA/ARTEMIS software based on the Feff code, and referenced to pure metal standards placed downstream of the sample between ionization chamber 1 and ionization chamber 2.

This experiment looked at two different cathode electrocatalysts made by BASF E-TEK, one being 20 wt% Pt nanoparticles supported on high surface area Vulcan XC-72 carbon and the other 30 wt% PtCo nanoparticles supported on high surface area Vulcan XC-72 carbon support. The membrane electrode assembly consisted of a Nafion® 115 polymer electrolyte membrane between the two electrodes. The gasket configuration on each side was identical, a 25 μm , 50 μm and 200 μm gasket, moving away from the center. This setup was sandwiched in between precision machined graphite blocks, containing single serpentine flowfield gas flow channels. The cell was completed with gold plated electrical end blocks that were also machined to contain a window at the point of X-ray passage. The cells were constructed according to USFCC protocol [4]. The Pt-Pd MEAs consisted of a 2.25 cm x 2.25 cm electrode with 0.1 mg/cm² of 30 wt% Pd on the anode and 0.1 mg/cm² of 20 wt% Pt on the cathode. The PtCo-Pd MEAs were a binary alloy cathode containing 0.1 mg/cm² of 30 wt% PtCo and 0.1 mg/cm² of 30 wt% Pd on the anode. Pd anodes were used in this experiment to help isolate the cathode electrocatalyst as Pt anodes would have produced additional unwanted absorption in transmission, complicating the bulk signal.

All gases used were of 99.9999% purity. During initial fuel cell warm-up, prior to operation, the gas fuels were <3.65% H₂ in He (Regen gas) on the anode and reactant grade Ar on the cathode. Once the conditioning phase protocol was initiated, the gas feeds were switched to reactant grade H₂ on the anode and reactant grade air on the cathode as the source for O₂. The gas fuels were heated at two separate locations on each line, first during humidification in the humidifiers and second in-line between the humidifiers and the fuel cell. The gaseous fuel was bubbled through the humidifiers to bring it to reactant temperature, about 5 °C below the cell temperature, and to humidify the gas, as a hydrated membrane is necessary for conduction protons and carrying out the reaction. Both the anode and cathode streams were held at 100% relative humidity to maintain a sufficient hydration cell. After travelling through the humidifiers, the gas fuels flowed through heated lines to the cell. The heating of these lines was designed to maintain the temperature of the gas and prevent water condensation that is neither beneficial to X-ray spectroscopy nor to cell performance. The gaseous fuels were pumped through the cell at flow rates corresponding to a 2:1 hydrogen:oxygen stoichiometry. The cell temperature was also recorded and maintained at a steady level for the duration of the

	Pt-Pd MEA, #1	Pt-Pd MEA, #2	PtCo-Pd MEA, #1	PtCo-Pd MEA, #2
Cell Temperature (°C)	79.5	64	66	62
Cathode Humidifier (°C)	74.5	64	64.5, Increased to 72 near end	62
Anode Humidifier (°C)	74	65	65.5, Increased to 70 near end	64
Cathode In-line Humidifier to cell (°C)	79.5	61, Increased to 90 near end	87, Decreased to 72 near end	75
Anode In-line Humidifier to cell (°C)	79.5	59, Increased to 80 near end	83, Decreased to 67 near end	73
H ₂ flow rate (mL/min)	Increased from 46 to 168	73	73	73, Increased to 146 for several scans, then returned to 73
H ₂ back pressure (psi)	Increased from 3.8 to 18.8	5	4.5	6
Air flow rate (mL/min)	Increased from 176 to 555	216	211	211
Air back pressure (psi)	Increased from 9.4 to 19.6	8	9	9

Table 2. General cell conditions, including temperature and gas flow rate and back pressure, for each of the four MEAs tested.

experiment. All temperatures were recorded. See Table 2 for the temperatures and flow rates of each of the MEAs tested.

Tested cells were conditioned according to the break-in period protocol developed by the USFCC [4]. Other load programs were performed on the cells including: square wave sequences (30 seconds at 0.6 V, 30 seconds at 0.96 V), constant current operation (at varying loads), and sequences where the cell was cycled between 0.5 V and 1.4 V for an hour and then bulk electrolysis was run at 1.4 V followed by 0.5 V. The high frequency impedance (HFI) of the MEAs was determined before and after cell conditioning and testing using A.C. impedance spectroscopy. Cyclic Voltammetry (CV) was performed on the cell using Corrware. The CV, bulk electrolysis and A.C. impedance were performed with a 1260A Impedance/Gain-Phase Analyzer and a 1287A Potentiostat (Solartron). See Table 3 for a description of the load sequences implemented with each MEA.

	Pt-Pd MEA, #1	Pt-Pd MEA, #2	PtCo-Pd MEA, #1	PtCo-Pd MEA, #2
Before Stage 1	N/A	N/A	Pol. curve	OCP for 1hr
Stage 1	0.6 V	0.6 V	0.6 V	0.6 V
Stage 2	0.7 V, 0.5 V for 9 cycles	0.7 V, 0.5 V for 9 cycles	0.7 V, 0.5 V for 9 cycles	0.7 V, 0.5 V for 9 cycles
After Stage 2	Pol. curve then 1 hr at OCP. Polarization curve then 1 hr at 1 amp, repeat	1 amp for 45 min, Pol. curve, 1 amp for 1 hr, 3 Pol. curves, 6 1-hr square wave sequences	2 Pol. curves — cycle down then up potential, constant current at 2 amps for 2.5 hr, 2 1-hr square wave sequences	1 hr at 1 amp, 2 hr at 3 amps, Pol. curve, bulk electrolysis at 0.5 V then 1.4 V for 3 cycles

Table 3. Electrical sequences implemented for each MEA, including voltage or current setting and length of time for each step. Polarization curve is abbreviated as Pol. curve. The square wave sequence consisted of 30 second steps at 0.6 V and 0.96 V.

RESULTS

Cell parameters were monitored throughout the experiment and maintained at constant values within experimental constraints, with the goal of minimizing the active variables in the experiment. The first Pt-Pd MEA study was abbreviated due to poor electrical performance, operating at a maximum of 0.46 amps/cm² at 0.1 V, with the H₂ flow rate at 168 mL/min with a back pressure of 18.8 psi, air flow rate at 555 mL/min with a back pressure of 19.6 psi and the cell torqued to 110 psi. The HFI of the cell was 0.15 ohms, approximately an order of magnitude higher than expected. The second Pt-Pd MEA was then tested, yielding a much better performance. The second Pt-Pd MEA achieved a performance of 0.97 amps/cm² at 0.1 V, with the H₂ flow rate at 73 mL/min with a back pressure of 4.3 psi, and the air flow rate at 211 mL/min with a back pressure of 7.9 psi. The final HFI read 0.057 ohms. The first PtCo-Pd MEA showed lower performance as compared to the second Pt-Pd MEA. The first PtCo-Pd MEA was the first to exhibit negative response to the conditioning phase protocol. A polarization curve before conditioning demonstrates the cell performance to be operating at 0.90 amps/cm² at 0.1 V, while a polarization curve after the conditioning phase displayed cell performance to be 0.65 amps/cm² at 0.1 V with an HFI of 0.059 ohms. The second PtCo-Pd

MEA demonstrated the expected performance increase during the conditioning phase. A polarization curve after stage 2 shows the cell performing at 0.90 amps/cm² at 0.1 V with an HFI of 0.058 ohms. Table 4 provides a summary of the electrochemical data for each MEA.

	Max Performance (amps/cm ²)	HFI, before test (ohms)	HFI, after test (ohms)
Pt-Pd MEA, #1	0.46	N/A	0.15
Pt-Pd MEA, #2	0.97	0.0768	0.057
PtCo-Pd MEA, #1	0.65	0.077	0.059
PtCo-Pd MEA, #2	0.90	N/A	0.056

Table 4. Electrochemical data for each MEA, including the maximum performance of each cell in amps/cm² (data shown is for 0.1 V) and the HFI before and after testing.

The fluorescence and transmission spectra were analyzed as a function of time. This research concentrates on the variations within the edge step of the spectra. This can lead to information concerning the behavior and environment of the PEFCs with regard to humidity and catalyst loss or modification (an increase in particle size for example). Both the fluorescence and transmission spectra demonstrate a decrease in edge step over time in general, but do have several spectra that do not fit this trend. During both of the Pt-Pd MEAs and both of the PtCo-Pd MEAs, several XAFS scans had to be discarded due to glitches in the XAFS spectra, which likely arose from condensed water bubbles in transition through the cell. The PtCo-Pd MEA tested at the Co-K edge consistently experienced glitches at about 8.3 keV while the glitches in the Pt-Pd MEAs were less localized, occurring just before and after the absorption edge and throughout the XAFS tail as well.

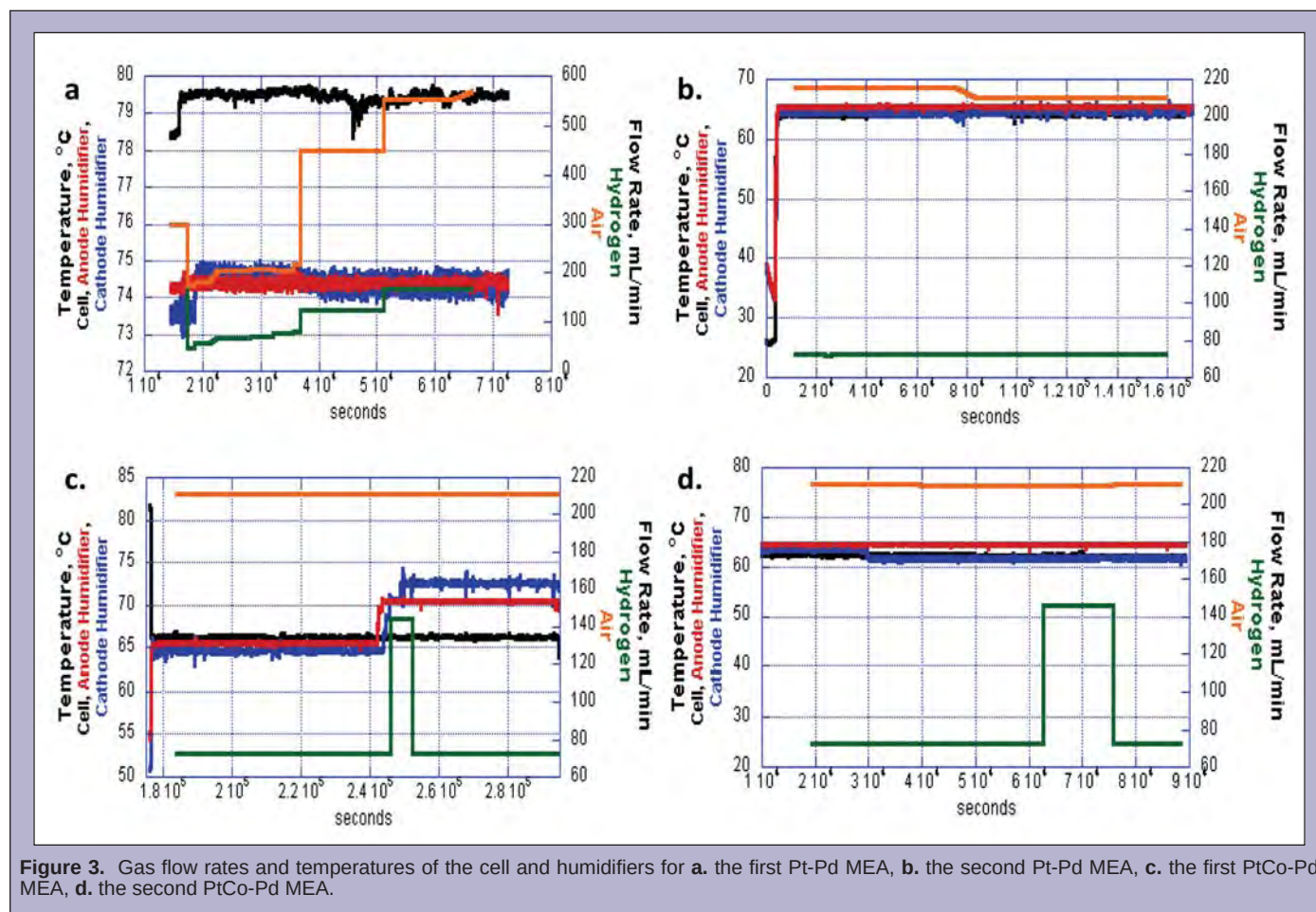
DISCUSSION

The stable gas flow rates and cell and humidifier temperatures (Figure 3) indicate that observed catalyst loss and cell performance are not functions of these temperature parameters and thus more likely functions of either the electrical parameters in the conditioning phase or of the changing MEA environment with regard to water volume at the electrodes and in the PEM. Figure 4 shows fluorescence spectra from each of the four MEAs. A decrease of the EXAFS region indicates continual loss of fluorescing/absorbing material from the cathode, which is clearly present for the Pt-Pd MEAs as shown in Figure 4(a,b). Detailed scan to scan observations suggest that the water volume of the electrodes is dynamic, experiencing both increases and decreases as discussed later, but is consistent with a continual decrease in the fluorescence as a loss of Pt from the cathode. This continual decrease is not as clear in the spectra for the PtCo-Pd MEAs, suggesting that those MEAs are experiencing less catalyst loss. This is supported by examining the percent change in the edge step over time. The first Pt-Pd MEA ended at a fluorescence edge step that was 87.6% of the initial edge step and the second Pt-Pd MEA ended with a fluorescence edge step that was 79.0% of the original. Both PtCo-Pd MEAs increased, ending at 120.7% and 167.0% of the original, for the first and second respectively, which corroborates with the idea of low PtCo loss. The overall increase in the PtCo edge steps for each MEA arose from the water volume decreasing at the cathode during the 1.4 V bulk electrolysis steps. This trend is

present in both the Pt-L₃ edge spectra and the Co-K edge spectra. A look at the transmission spectra for all four MEAs shows a decrease in the height of the edge step. Because the decrease in the edge step is not present in the fluorescence spectra, the cause must be loss of material from the anode. As water has already been ruled unlikely due to the fluctuations observed, the decrease of the entire spectra suggests loss of Pt, Pd and/or carbon support. Loss of Pt would also be consistent with a decreasing edge step, however, as mentioned previously, the MEAs with PtCo cathodes actually showed increased Pt fluorescence, which is not consistent with Pt loss. The evidence thus suggests that the increased Pt transmission results from loss of Pd from the anode or support loss from either electrode.

The thrust of the analysis for this experiment examines the fluorescence and transmission edge steps, as they contain information regarding the changing MEA environment on a scan to scan basis. Figure 5 shows plots of the fluorescence and transmission edge steps plotted against time along with the potential and current for each of the MEAs tested. As described in Table 1, opposing changes in the edge step show correlation between the anode and cathode with respect to water activity. This correlation is clear in the second Pt-Pd MEA and in the PtCo-Pd MEAs but not in the first Pt-Pd MEA. The first Pt-Pd MEA demonstrated a high HFI and poor performance (Figure 6) compared to other MEAs as well, suggesting that it was running at a state of low relative humidity and was drying out, yielding the poor performance as protons are less able to traverse the PEM and reach the cathode. The second Pt-Pd MEA and both

PtCo-Pd MEAs obtained low HFI readings, meaning there was low resistance in those MEAs, suggesting that the cells are operating at high relative humidity. A cell functioning at a high relative humidity, as long as flooding, which can be detrimental to cell performance, has not occurred, would be less affected by the production rate of water within the cell and less likely to show major fluctuation in water activity as a function of changing electrical parameters. This would result in an increased correlation between the fluorescence and transmission edge steps as the changing water level would be more closely related to humidity levels of the gas stream than of the amount of H₂O produced from the combination of protons and oxygen anions. The correlation between fluorescence and transmission edge steps along with the correlation between relative humidity and cell performance indicates that the conditioning phase has a component arising as a function of humidity, i.e., a period in which the cell becomes properly humidified so as to achieve optimized and stable performance.



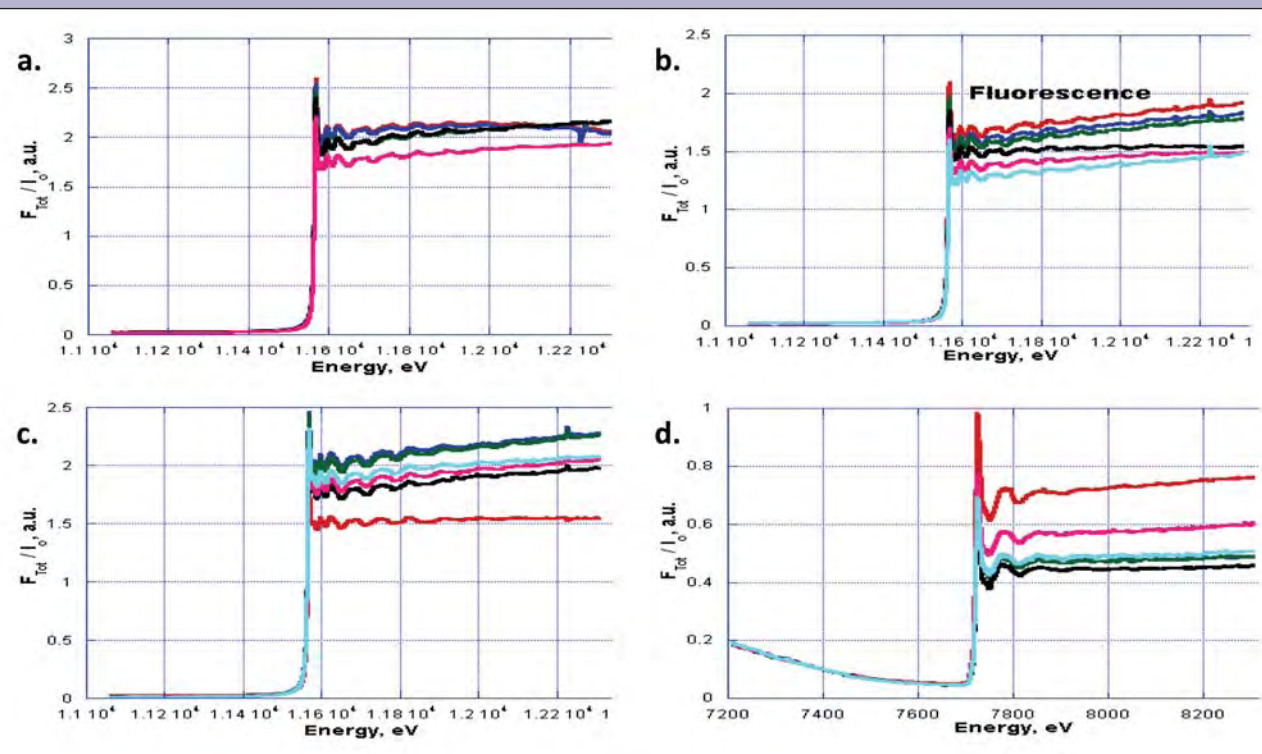


Figure 4. Fluorescence spectra over time for **a.** the first Pt-Pd MEA, **b.** the second Pt-Pd MEA, **c.** the first PtCo-Pd MEA, **d.** the second PtCo-Pd MEA. The color scheme in each graph is consistent with time (Red→Blue→Green→Black→Pink→Teal represents increasing time). The decrease in the EXAFS portion of the Pt-Pd MEA spectra indicates a continual loss in Pt. Note the lack of a downward trend with the PtCo spectra, suggesting less catalyst loss in the PtCo-Pd MEAs.

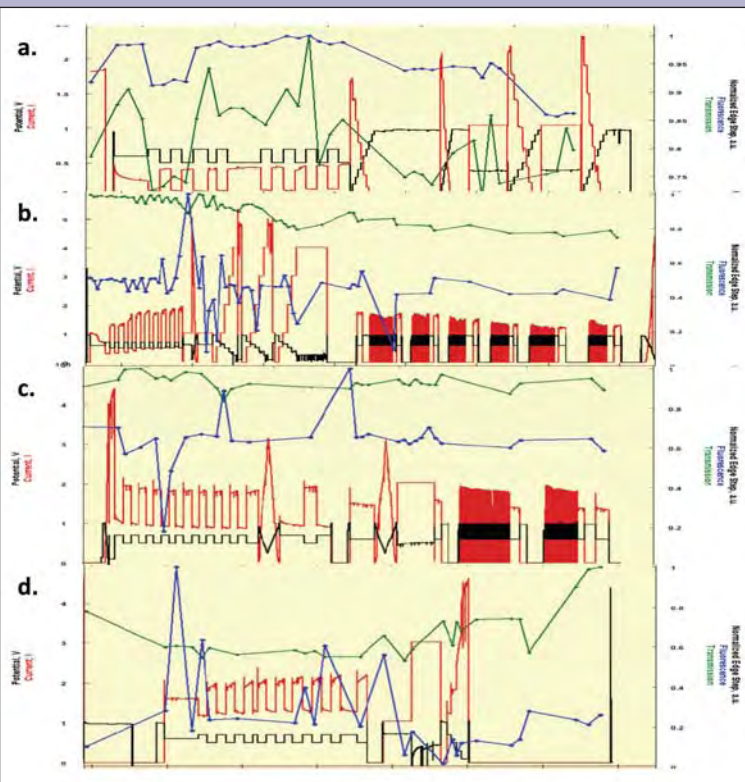


Figure 5. Fluorescence and transmission edge steps plotted against time along with the voltage and current sequences for **a.** the first Pt-Pd MEA, **b.** the second Pt-Pd MEA, **c.** the first PtCo-Pd MEA, **d.** the second PtCo-Pd MEA.

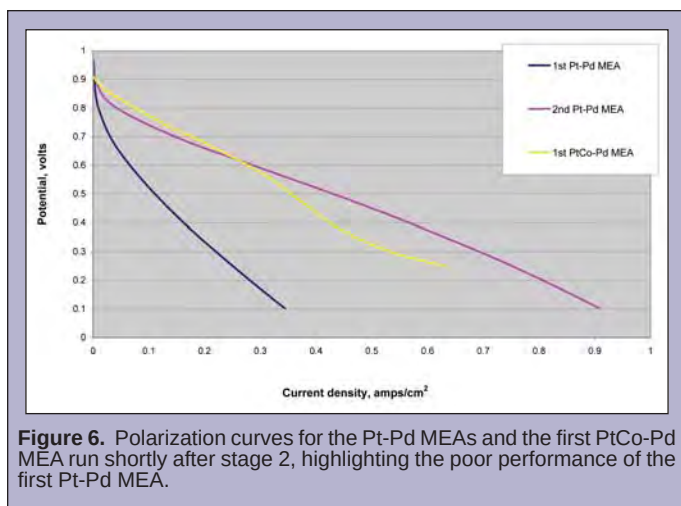


Figure 6. Polarization curves for the Pt-Pd MEAs and the first PtCo-Pd MEA run shortly after stage 2, highlighting the poor performance of the first Pt-Pd MEA.

CONCLUSION

The good correlation between the fluorescence and transmission edge steps in cells that performed well combined with the correlation between low HFI and improved cell performance gives preliminary evidence that cell conditioning is a function of humidity in the cell. This finding agrees with previous work stating the importance of good relative humidity on cell performance [7]. Note that these findings do not indicate that the more water the better, as flooding of the cell with too much water is a major issue, leading to poor reactant transport in the electrode layers and corrosion of the catalysts and supports within the fuel cell [7].

In testing both Pt-Pd MEAs and PtCo-Pd MEAs, the consistent decrease of the fluorescence edge step with the Pt-Pd MEAs as opposed to the rather consistent edge step with the PtCo-Pd MEAs suggests that PtCo/C may be a more durable electrocatalyst than Pt/C alone. However, the authors caution that a more thorough effort is required to fully substantiate this postulate.

There is undoubtedly more understanding of the conditioning phase that can be gained from further research. Further analysis of the EXAFS will give a better understanding of the atomic environment, including information on the coordination of Pt and interactions between the electrocatalyst and oxygen. Further experimentation should be completed to observe particle size during the conditioning phase, verifying whether loss of catalyst in the beam is actually catalyst getting washed from the electrode or if it is a function of catalyst rearrangement and growth in particle size.

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Kiran Rangaraj participated in the CCI program during the summer of 2008, where he studied protein-protein interactions involved in multiple DNA repair mechanisms in the Life Sciences Division at Lawrence Berkeley National Laboratory (LBNL). Kiran presented the work he completed there at the inaugural 2008 DOE Science and Energy Research Challenge. Kiran is currently continuing his studies at LBNL while pursuing an undergraduate degree in biochemistry at the University of California–Berkeley. He plans to enter into a graduate school program following his graduation. Kiran grew up in Milpitas, CA, and he enjoys drawing, weight training, and mountain biking.

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WHERE MULTIFUNCTIONAL DNA REPAIR PROTEINS MEET: MAPPING THE INTERACTION DOMAINS BETWEEN XPG AND WRN

KIRAN RANGARAJ, PRISCILLA K. COOPER AND KELLY S. TREGO

ABSTRACT

The rapid recognition and repair of DNA damage is essential for the maintenance of genomic integrity and cellular survival. Multiple complex and interconnected DNA damage responses exist within cells to preserve the human genome, and these repair pathways are carried out by a specific interplay of protein-protein interactions. Thus a failure in the coordination of these processes, perhaps brought about by a breakdown in any one multifunctional repair protein, can lead to genomic instability, developmental and immunological abnormalities, cancer and premature aging. This study demonstrates a novel interaction between two such repair proteins, Xeroderma pigmentosum group G protein (XPG) and Werner syndrome helicase (WRN), that are both highly pleiotropic and associated with inherited genetic disorders when mutated. XPG is a structure-specific endonuclease required for the repair of UV-damaged DNA by nucleotide excision repair (NER), and mutations in XPG result in the diseases Xeroderma pigmentosum (XP) and Cockayne syndrome (CS). A loss of XPG incision activity results in XP, whereas a loss of non-enzymatic function(s) of XPG causes CS. WRN is a multifunctional protein involved in double-strand break repair (DSBR), and consists of 3'–5' DNA-dependent helicase, 3'–5' exonuclease, and single-strand DNA annealing activities. Nonfunctional WRN protein leads to Werner syndrome, a premature aging disorder with increased cancer incidence. Far Western analysis was used to map the interacting domains between XPG and WRN by denaturing gel electrophoresis, which separated purified full length and recombinant XPG and WRN deletion constructs, based primarily upon the length of each polypeptide. Specific interacting domains were visualized when probed with the secondary protein of interest which was then detected by traditional Western analysis using the antibody of the secondary protein. The interaction between XPG and WRN was mapped to the C-terminal region of XPG as well as the C-terminal region of WRN. The physical interaction between XPG and WRN links NER, (made evident by the disease XP) with DSBR, which imparts additional knowledge of the overlapping nature of these two proteins and the previously distinct DNA repair pathways they are associated with. Since genomic integrity is constantly threatened by both endogenous and exogenous (internal and external) damage, understanding the roles of these proteins in coordinating DNA repair processes with replication will significantly further understanding how defects instigate physiological consequences in response to various DNA damaging sources. This ultimately contributes to our understanding of cancer and premature aging.

INTRODUCTION

The human genome is constantly subjected to both endogenous and exogenous (internal and external) damage from cellular metabolism, environmental sources of ultraviolet (UV) and ionizing radiation, and mutagenic chemicals, which generate several kinds of lesions throughout cellular DNA. Natural by-products of oxidative phosphorylation in mitochondria in addition to other cellular processes of the cell generate reactive oxygen species, which are estimated to produce 50 000–100 000 oxidative DNA lesions per mammalian cell per day, each of which could potentially cause errors in DNA replication or transcription if not repaired [1]. Such lesions may elicit point mutations or chromosomal rearrangements, prompt single-strand (ssDNA) or double-strand (dsDNA) breaks in DNA during replication, or trigger a stress response via a signal transduction pathway, all known precursors to premature aging, cancer and a number of genetic diseases. The rapid recognition and repair of DNA damage is essential for the maintenance of genomic integrity and cellular survival [2]. Multiple DNA repair pathways have evolved within cells to provide a distinct but overlapping capacity to recognize and excise lesions, in coordination with other necessary cellular processes of DNA replication, transcription and recombination such that the human genome is preserved [1]. However, the coordination of DNA repair processes may be compromised by a breakdown in any one of the numerous multifunctional proteins involved in initiating and mediating communication between repair and replication pathways, ultimately compromising the ability to restore genomic integrity. Elucidating the precise biological roles of these proteins has become an important challenge since a number of diseases and conditions have been either directly linked or associated with defects in certain repair proteins. Much of cancer and aging research focuses on understanding the involvement of these proteins within necessary repair pathways, in order to identify the exact molecular mechanisms that trigger inherited defects in DNA repair.

Ultraviolet radiation is recognized as an important health risk to the human population as noted by an ongoing epidemic of skin cancer [3]. The biochemical pathway of nucleotide excision repair (NER) is the primary mechanism in mammalian cells to remove the bulky DNA helix-distorting lesions that are caused by UV light. Eukaryotic NER can be subdivided into two subpathways — global genome repair (GGR), which removes lesions from all regions of the genome, and transcription coupled repair (TCR), which involves accelerated removal of damage from actively transcribed strands of genes [4]. The importance of GGR and TCR is attested by the existence of dramatic inherited diseases such as Xeroderma pigmentosum (XP), Trichothiodystrophy (TTD), and Cockayne syndrome (CS) [5].

Much research has focused on XP, which is an autosomal recessive genetic disorder where patients carry mutations that partially or totally impair the efficiency of NER processes [5]. XP patients lack essential repair pathways by which the cell can remove the vast majority of UV-induced DNA damage, thus clinical features of XP include extreme sun sensitivity with marked thickening of the skin, alterations in pigmentation, and a high incidence of skin malignancies at a young age. XP patients can be subdivided into seven complementation groups XP-A through XP-G, plus one variant form XP-V, depending on which gene is affected. Each complementation group XP-A to XP-G represents separate proteins that are involved in the first steps of the NER pathway (damage recognition and incision-excision) and interact together to form recently mapped interactions with other proteins. One such gene of the complementation group G encodes for the protein XPG, which is a vital multifunctional protein currently under focus at the Cooper Lab of the Life Sciences Division at Lawrence Berkeley National Laboratory (LBNL).

XPG protein is a junction-specific endonuclease that incises the damaged DNA strand 3' to the lesion undergoing repair [6]. The enzyme cleaves model DNA bubble structures specifically near the junction of unpaired DNA with a duplex region. Structurally, XPG shares extensive sequence homology with another structure-specific endonuclease, flap endonuclease 1 (FEN-1), exclusively through the N and I domains that together form the nuclease active site (Figure 1A). The endonuclease activity is vital to the repair of UV-damaged DNA by NER, since point mutations within XPG inactivate this function and result in XP.

XPG is structurally unique in that the endonuclease domains are separated by a "recognition" (R) domain and a "carboxyl" (C) terminus which impart XPG with additional functional abilities. Truncation mutations in XPG are more severe, resulting in a combined disease of XP with the developmental disorder Cockayne syndrome (CS), in which patients display profound postnatal neurological and developmental dysfunction, premature aging, and severe wasting that becomes evident and lethal within the first few years of life (Figure 1B). The disease severity strongly suggests that non-enzymatic functions of XPG are essential to normal

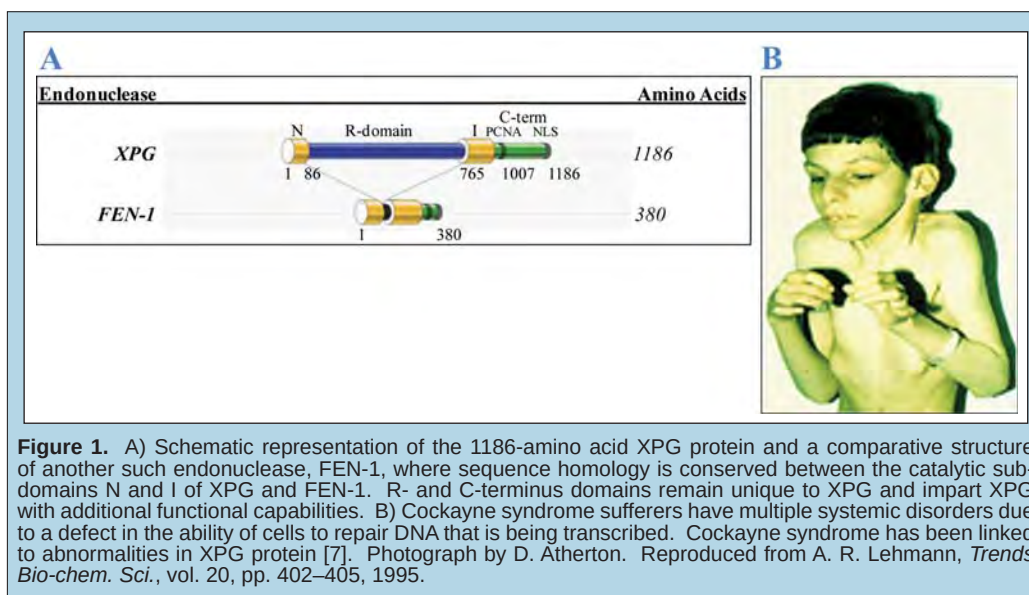


Figure 1. A) Schematic representation of the 1186-amino acid XPG protein and a comparative structure of another such endonuclease, FEN-1, where sequence homology is conserved between the catalytic subdomains N and I of XPG and FEN-1. R- and C-terminus domains remain unique to XPG and impart XPG with additional functional capabilities. B) Cockayne syndrome sufferers have multiple systemic disorders due to a defect in the ability of cells to repair DNA that is being transcribed. Cockayne syndrome has been linked to abnormalities in XPG protein [7]. Photograph by D. Atherton. Reproduced from A. R. Lehmann, *Trends Bio-chem. Sci.*, vol. 20, pp. 402–405, 1995.

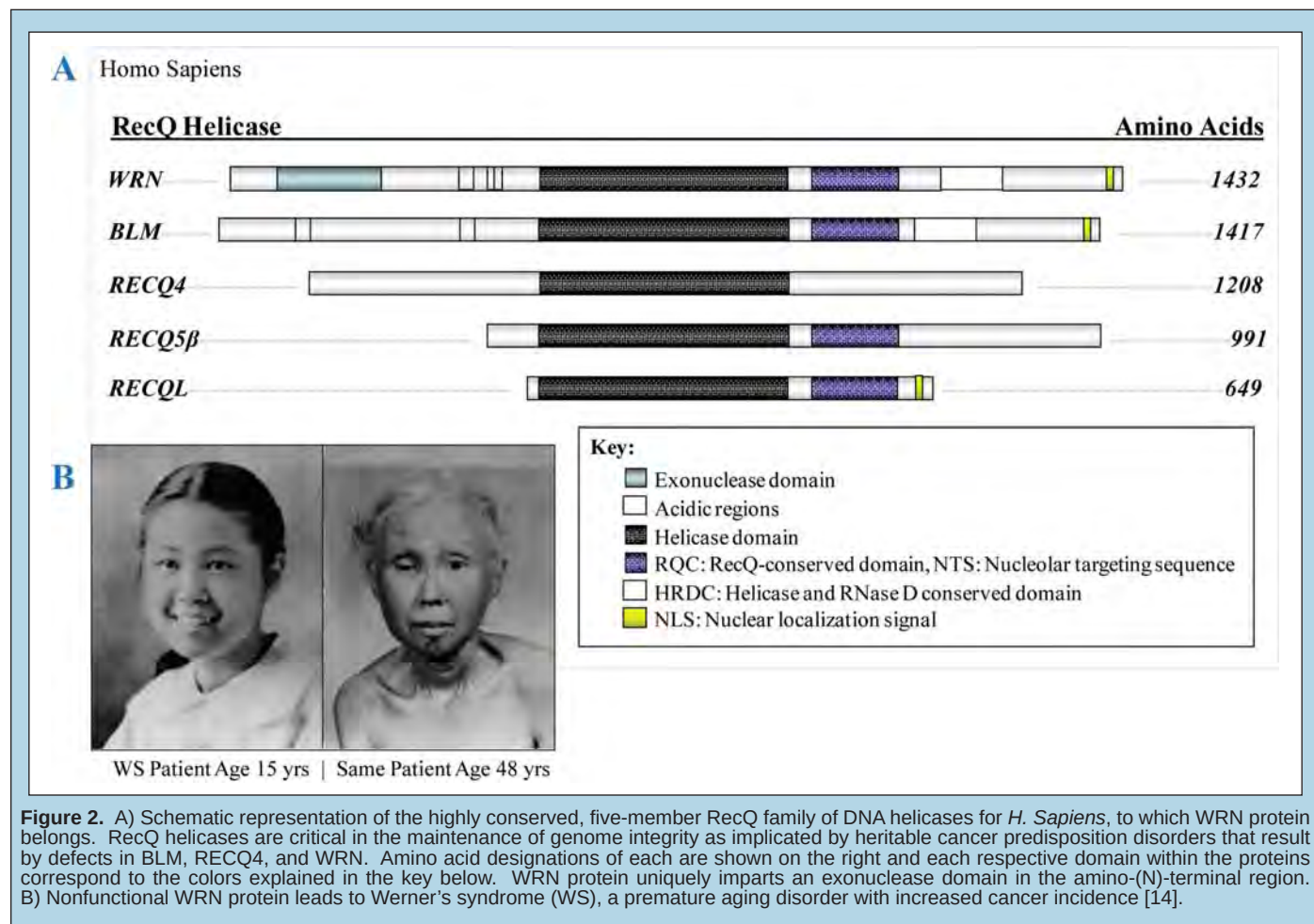
postnatal development. Scientists at the Cooper Lab have recently identified novel structural roles of the protein in both TCR and base excision repair (BER) of oxidative damage [8], [9], [10] (Cooper Lab, unpublished results). BER is a critical lesion-amending pathway involving the repair of oxidative DNA base modifications, deaminated or alkylated bases, apurinic/apyrimidic (AP) sites, and ssDNA breaks [11]. Recent studies have also suggested that XPG may have a novel replication-associated function and that it communicates with proteins known to be involved in signaling and processing of stalled or collapsed DNA replication forks and double strand break repair (DSBR), thereby extending its role in DNA damage response (Cooper Lab, unpublished results). Novel XPG binding partners were assessed using a combination approach of proteomic analysis and directed searching, and this assessment identified several proteins including Rad51, the Mre11-Rad50-Nbs1 (MRN) protein complex, as well as Werner (WRN) and Bloom (BLM) syndrome helicases, that are each functionally involved at stalled or collapsed replication forks.

One of the proteins identified was WRN, a 160 kDa (1432-amino acid) member of the RecQ category of helicases, which are enzymes that separate the complementary strands of nucleic acid duplexes using the energy derived from adenosine triphosphate (ATP) hydrolysis [12]. RecQ helicases represent a highly conserved, five-member family that is required for the maintenance of genome integrity. This integrity is implicated by heritable cancer predisposition disorders that result from defects in any of three

RecQ family members (BLM, WRN, and RecQ4) (Figure 2A) [13]. Patients lacking functional WRN protein have Werner syndrome (WS), an autosomal recessive disorder characterized at the cellular level by genomic instability. Clinical features of WS include numerous prematurely developed age-related pathologies, short stature, leg ulceration, soft-tissue calcification, and increased cancer incidence (Figure 2B). WRN has an unusual preference for unwinding DNA substrates with extensive secondary structure, such as Holliday Junctions (HJ), as well as bubbles, forks, and D-Loops, all functional intermediates in the homologous recombination repair (HRR) subpathway of DSBR. Unlike other RecQ helicases, WRN additionally possesses 3'–5' exonuclease activity [15], [16].

Recent data demonstrates that XPG strongly binds HJ substrates, and that the presence of XPG increases the binding of WRN to the DNA (K. Trego, Cooper Lab, unpublished results). The functional significance of this physical interaction was examined by testing the WRN helicase activity on a dsDNA substrate with overhanging ends. Interestingly, XPG strongly stimulated the helicase activity of WRN which, coupled with all of the other findings, suggests that the physical interaction of XPG with WRN may be important in coordinating a possible replication-associated function of XPG at stalled or collapsed replication forks with ds breaks (K. Trego, Cooper Lab, unpublished results).

Cooper Lab studies have demonstrated that XPG physically interacts with WRN protein in vivo. Therefore, this study used Far Western analysis to further examine the direct interaction of these



two proteins *in vitro*, since *in vivo* interactions may be mediated via an accessory protein [17], [18]. The Far Western technique allowed mapping of the precise domains between XPG and WRN proteins that are responsible for this novel interaction. The analysis involved separating full length and recombinant XPG and WRN deletion constructs based primarily upon the length of each polypeptide through denaturing gel electrophoresis. Thus, specific interacting domains could be visualized when probed with the secondary protein of interest. Results defined, for the first time, interaction domains between XPG and WRN that have imparted additional knowledge on the multifunctional role these proteins play in the maintenance of genomic stability.

MATERIALS AND METHODS

Buffers

6X Sodium Dodecyl Sulfate (SDS) Sample Buffer was prepared using 70% 0.5 M Tris, pH 6.8, and 30% glycerol, with 0.35 M SDS, 0.6 M (D,L)-1,4-dithiothreitol (DTT) from Soltec Ventures, Inc., and 0.18 mM Bromophenol Blue dye (BPB). Reagents were combined in a 50 mL conical flask, then vortexed prior to being stored at -20 °C in 1 mL aliquots. All reagents excluding DTT were purchased from Sigma-Aldrich Corporation.

5X Tris-Glycine SDS Running Buffer for SDS Polyacrylamide Gel Electrophoresis (PAGE) was prepared using deionized water with 125 mM Tris-base, 0.96 M glycine from Bio-Rad Laboratories, Inc., and 17 mM of SDS. One liter of the 5X stock was made, from which dilutions to 1X were performed prior to gel running.

Standard Tris-Glycine Transfer Buffer for SDS-PAGE was prepared using deionized water containing 20% methanol, with 25 mM Tris-base and 190 mM glycine.

Proteins

Full length XPG protein and XPG protein domains were purified in the Cooper Lab as previously described or were obtained from Miaw-Sheue Tsai of the Expression and Molecular Biology (EMB) Core (Life Sciences Division, LBNL, Berkeley, CA 94720) [19].

All full-length WRN fractions and WRN domain constructs were kindly provided by Steven M. Yannoni (Life Sciences Division, Department of Molecular Biology, LBNL, Berkeley, CA 94720), J. Jefferson P. Perry (Department of Molecular Biology and Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA 92037), and L. David Finger (City of Hope, Beckman Research Institute, Duarte, CA 91010). Protein purification was conducted as previously described [20]. Protein constructs were appended with an N-terminal His₆ tag, cloned into a vector and recombinantly overexpressed in bacterial or insect-cells. Cells were resuspended in Tris-HCl buffer (pH 7.5) and affinity-purified from sonicated cell lysate by conventional nickel-nitrilotriacetic acid agarose resin column chromatography. Subsequent column-chromatography methods were used to purify the protein constructs to near homogeneity.

Experimental Method

To obtain the Far Western Assay, 1.5–6.0 µg of each polypeptide (full-length, truncation and control proteins) was denatured by boiling for five minutes in a 1:6 volumetric dilution of 6X SDS-sample buffer upon a 95 °C heat block, then resolved by SDS-

PAGE using a precast 1.0 mm x 10 or 12 well, Novex® 4–12% or 4–20% Tris-Glycine Gel (Invitrogen Corp.). Molecular weight quantification of the proteins was achieved using Kaleidoscope Prestained Standards (Bio-Rad Laboratories). Proteins were transferred overnight to Bio-Rad Trans-Blot nitrocellulose filters using the corresponding Bio-Rad Mini Trans-Blot Electrophoretic Transfer Cell at 4 °C, after which the filters were briefly immersed in 1X Phosphate Buffered Saline (PBS) (Omni Pur) then Ponceau S Solution (Sigma-Aldrich) to provide temporary protein visualization and gauge the efficiency of transfer. Brief subsequent immersions in PBS allowed destaining of the background for increased visual clarity. Filters were immersed twice in denaturation buffer (6 M guanidine-HCl in PBS) for 10 minutes and then incubated six times for 10 minutes each in serial dilutions (1:1) of denaturation buffer in PBS to allow progressive protein renaturation. Filters were blocked in PBS containing 5% nonfat powdered milk for three hours at room temperature to prevent non-specific background binding of the antibodies to the membrane, prior to being incubated in full-length XPG or WRN proteins (10.0 pmole/mL) in PBS supplemented with 0.5% powdered milk, 0.1 or 0.5% Tween-20 (Sigma-Aldrich), 1.0 mM DTT, and 0.5 mM phenylmethylsulfonyl fluoride (PMSF) overnight at 4 °C with gentle agitation. Following overnight incubation, the filters were extensively washed four times for 10 minutes each in PBS containing 0.1–1.0% Tween-20, after which conventional Western blotting was performed to detect the presence of WRN or XPG using mouse monoclonal 4H12 Ab-66606 α WRN (Abcam) at a 1/666 dilution, or mouse 8H7 Ab-1 α XPG (NeoMarkers) at a 1/5 000 dilution, respectively, as primary antibody. After a one-hour incubation with the primary antibody, the filters were washed three times for five to ten minutes each with PBS containing 0.1–0.5% Tween-20. Enhanced Chemiluminescent (ECL) anti-mouse IgG/horseradish peroxidase conjugate (GE Healthcare) was applied as secondary antibody at a 1/(10 000) dilution for 45 minutes and detected by ECL using either Thermo Scientific, SuperSignal West Pico, or GE Healthcare-Amersham, Advance Western Blotting Detection kits. Filters were then exposed to film (GE Healthcare-Amersham Hyperfilm ECL) at 1–30 second exposure times to obtain the best image. Certain amendments to the stated protocol are described in the figure legends where appropriate.

RESULTS

To identify the XPG protein domain that mediates the interaction with WRN, *in vitro*, a series of XPG deletion constructs were previously recombinantly expressed and purified using conventional column chromatography to near homogeneity (Figure 3A). Deletion constructs together isolate each domain region within XPG (N, R, I and C-terminal domains), in order to potentially identify a single key domain or group of domains required for the binding of WRN (Figure 3B). XPG constructs were immobilized to a nitrocellulose filter and stained for total protein visibility (Figure 3C). The filter was then incubated in buffer containing the second protein of interest, WRN, and then washed to remove any unbound protein. The presence of WRN was detected using conventional Western analysis with WRN antibodies (Figure 3C). When WRN was used to probe nitrocellulose bound full length XPG and XPG deletion constructs, an immunoreactive band was detected where full length XPG, the positive control Replication Protein A (RPA), and

constructs XFX and Exon-15 had migrated, as well as the positive control, Replication Protein A (RPA). A previously established interaction between WRN and RPA allows for the immunoreactive band of RPA to confirm the ability of WRN protein to bind to the filter and be detected by antibodies during the Western analysis. The interaction viewed between WRN and the XPG domain regions appeared to be specific, as WRN did not bind to the negative control protein, bovine serum albumin (BSA), which was run in parallel on

the same blot. WRN protein also did not bind to the XPG deletion constructs XPGΔC, XFXΔC, and R-domain.

Importantly, the Far Western analysis identified the binding of WRN to full-length XPG, XFX, and Exon-15 domains, which together isolate the C-terminus of XPG as the key interaction domain with WRN (Figures 3A, 3B, 3C). As the binding of WRN to the full-length protein was expected, more critical are the deletion constructs which maintain the interaction. The first interacting

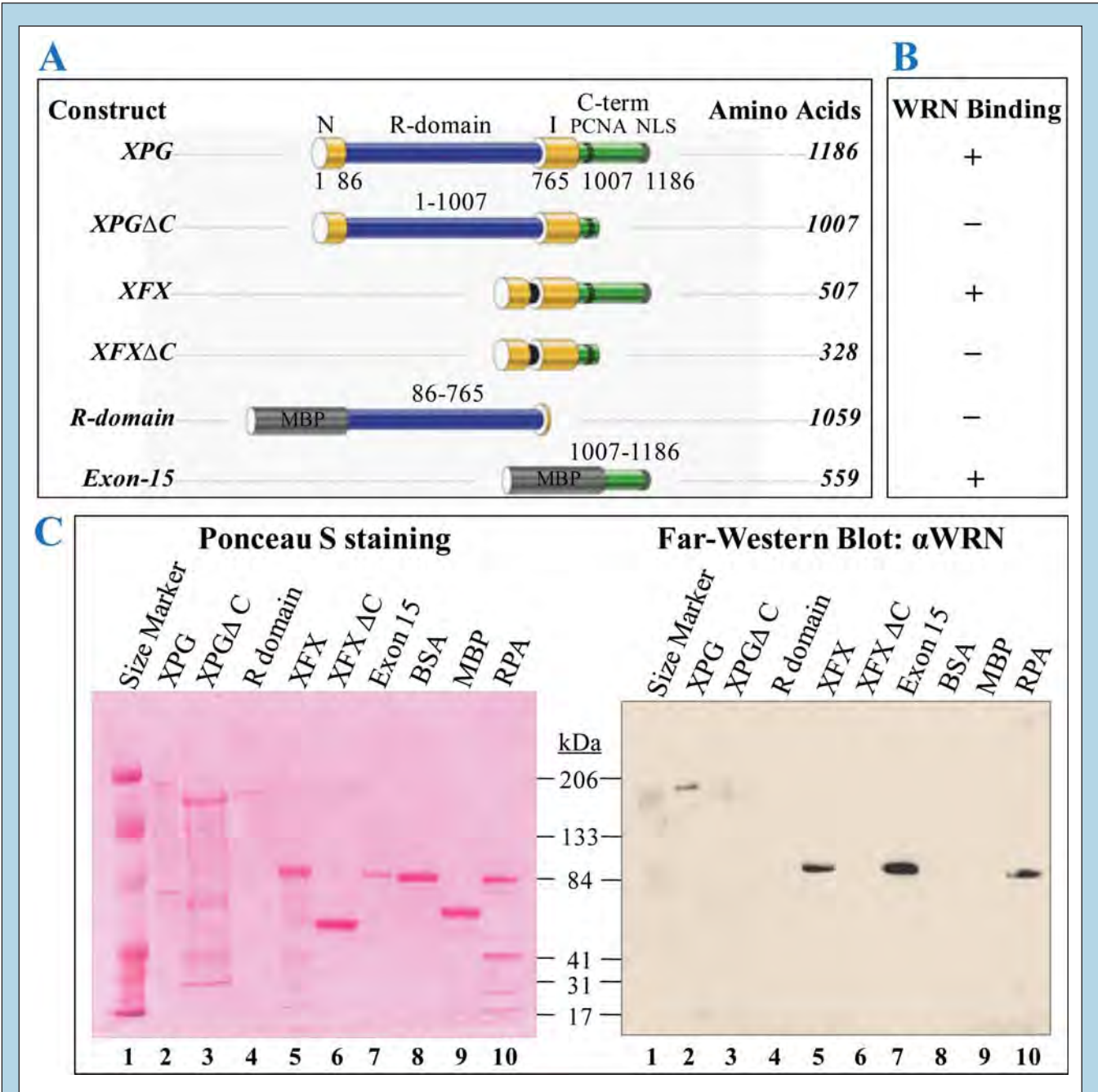


Figure 3. A) Series depiction of domain constructs applied for the interaction mapping with WRN. Protein constructs R-domain and Exon-15 are distinct from other constructs in that they are recombinant fusion peptides generated by fusing the N-terminal domains of the XPG construct with the C-terminus of a 42–3 kDa (380 amino acid) maltose-binding protein (MBP). This technique aided in the affinity purification process of the constructs. The numbers above each construct represent amino acid positions within full length XPG protein. B) Indication of the ability of each peptide to bind to WRN as detected by Far Western analysis. Deletion constructs XFX and Exon-15 maintain the interaction with WRN that is viewed with full length XPG protein. All other constructs fail to uphold WRN binding. C) Separated by 4–12% Tris-glycine SDS-PAGE and stained with Ponceau S Solution for temporary protein visualization, the purified constructs and control proteins BSA (– control), MBP (– control), and RPA (+ control) are shown on the nitrocellulose filter. To the right, protein-protein interaction between WRN and XPG deletion constructs are signaled by bands at designated migration areas on the filter following Western analysis using WRN antibody.

construct, XFX, preserves all domains of full-length XPG with the exclusion of the R-domain, which when coupled with the negative binding to the R-domain construct, indicates that the R-domain region is not required for WRN binding. Furthermore, Exon-15, a 559-aa deletion construct that comprises only the C-terminus (residues 1 007–1 186), bound to WRN and was found to be necessary and sufficient for interaction with WRN protein.

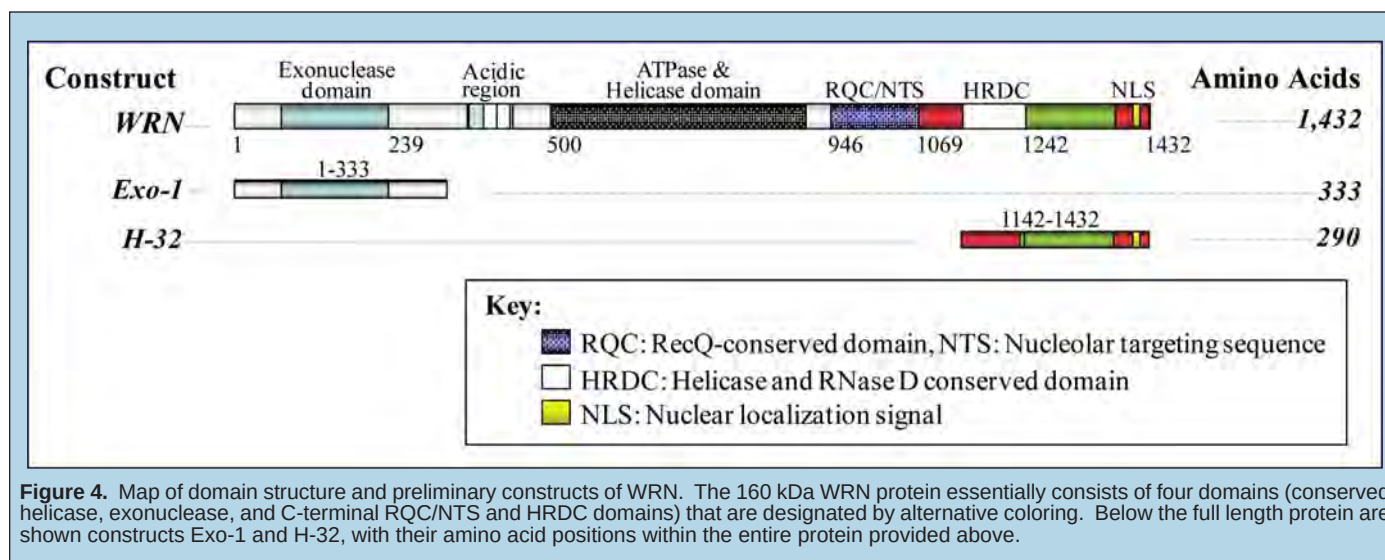
In order to further understand the nature of the XPG and WRN protein-protein interaction, in vitro, the regions of WRN protein that mediate the interaction with XPG were also sought. A reciprocal Far Western analysis was designed to meet this objective, and full-length XPG was used to probe nitrocellulose-bound WRN and recombinant WRN protein constructs (Figure 4). The WRN protein consists of four domains: 1) a central conserved helicase domain found in all RecQ helicases, 2) a unique N-terminal exonuclease domain, 3) a C-terminal region consisting of the RecQ-conserved domain/nucleolar targeting sequence (RQC/NTS) and 4) helicase and RNaseD conserved (HRDC) domains.

In addition to full-length WRN, preliminary Far Western assays included protein constructs, Exo-1, a peptide containing the exonuclease domain within residues 1–333, and H-32, which covers the final 290 residues of the 362 aa C-terminal region (Figures 4, 5A). Immunoreactive responses occurred as expected at sites where full-length WRN protein and the positive control proteins Cockayne Syndrome B (CSB), RPA, and full-length XPG had migrated. These signals confirm the efficiency of the incubation with XPG protein and Western probing with XPG antibody. In addition to these interactions, XPG binding to H-32 was found, but also for the negative control BSA, which was run parallel on the same blot along with another negative control protein, glutathione-S-transferase (GST) that showed no binding band. The interaction band with BSA confounds other results because it suggests a non-specific interaction due to error in the Far Western methodology. BSA had been applied as a negative control in previous Far Western assays of XPG constructs and had performed consistently (Figure 3C), which called into question the validity of the H-32 interaction band, which indicated the WRN C-terminus as being the domain responsible for the interaction with XPG. GST, however, performed as a negative

control which prompted further investigation into the cause of the interaction band with BSA.

To identify the basis for BSA reactivity, a second Far Western analysis was designed to examine whether the immunoreactive response to BSA was source-dependent. This was achieved by using two new sources of BSA along with the same WRN constructs and control proteins used in the previous Far Western analysis. Second sources of BSA were Standard BSA (1:10), in addition to an SDS-PAGE high-range protein standard (Bio-Rad, Cat. #161-0303), which contains a BSA molecular weight determinant for blotting applications with several other such protein markers (Figure 5B). Positive interactions among both new sources of BSA in this Far Western assay suggested non source-dependent reactivity and supported determining if the basis of the repeated immunoreactive response was due to a protein-protein interaction between XPG and BSA. This investigation was conducted by designing a control Far Western experiment (Figure 6A). The results demonstrated equivalent positive bands for four distinct sources of BSA, thereby eliminating the possibility of source-dependent reactivity. The results also showed that the positive signals were not due to interactions between BSA and XPG, since immunoreactive bands of equal intensity were found for BSA on the half of the control blot that had not been exposed to XPG. By eliminating the possibility of protein-protein interaction as being the cause for BSA reactivity, cross-reactivity between BSA and the antibodies used for the Western detection became the single unexamined cause. A second BSA control experiment was designed to isolate which antibody was causing the cross-reactivity with BSA (Figure 6B). The control experiment determined the primary 8H7 α XPG antibody as the cause for cross-reactivity, since sections two and four of the membrane only received secondary anti-mouse IgG/horseradish peroxidase conjugate and showed no such interaction. This result establishes that the BSA interaction band found in preliminary Far Western assays with WRN constructs were non-XPG dependent, validating the result that the WRN C-terminal construct, H-32, was interacting with XPG.

After the preliminary results were validated, a final Far Western analysis was designed to include six additional WRN C-terminal



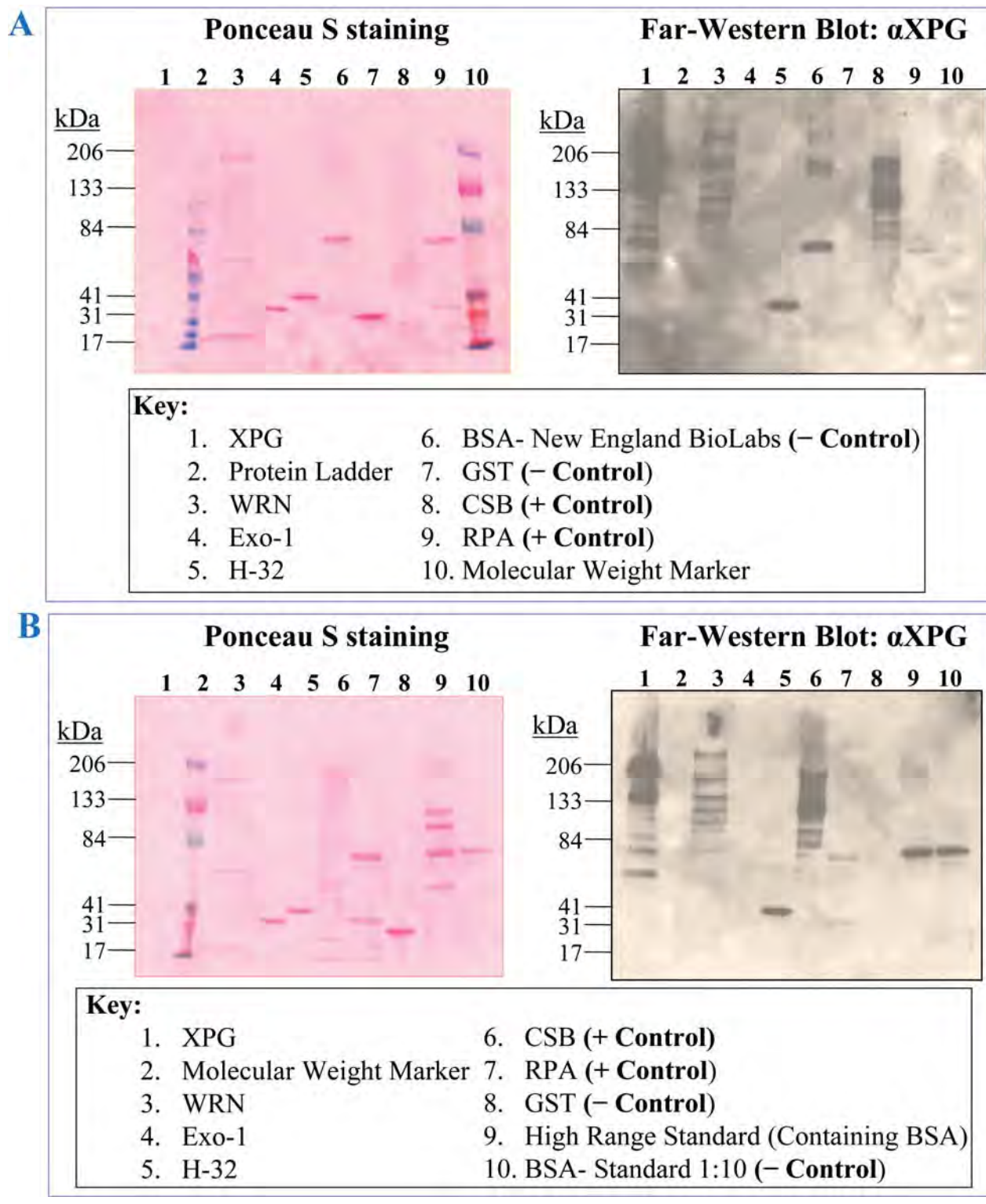
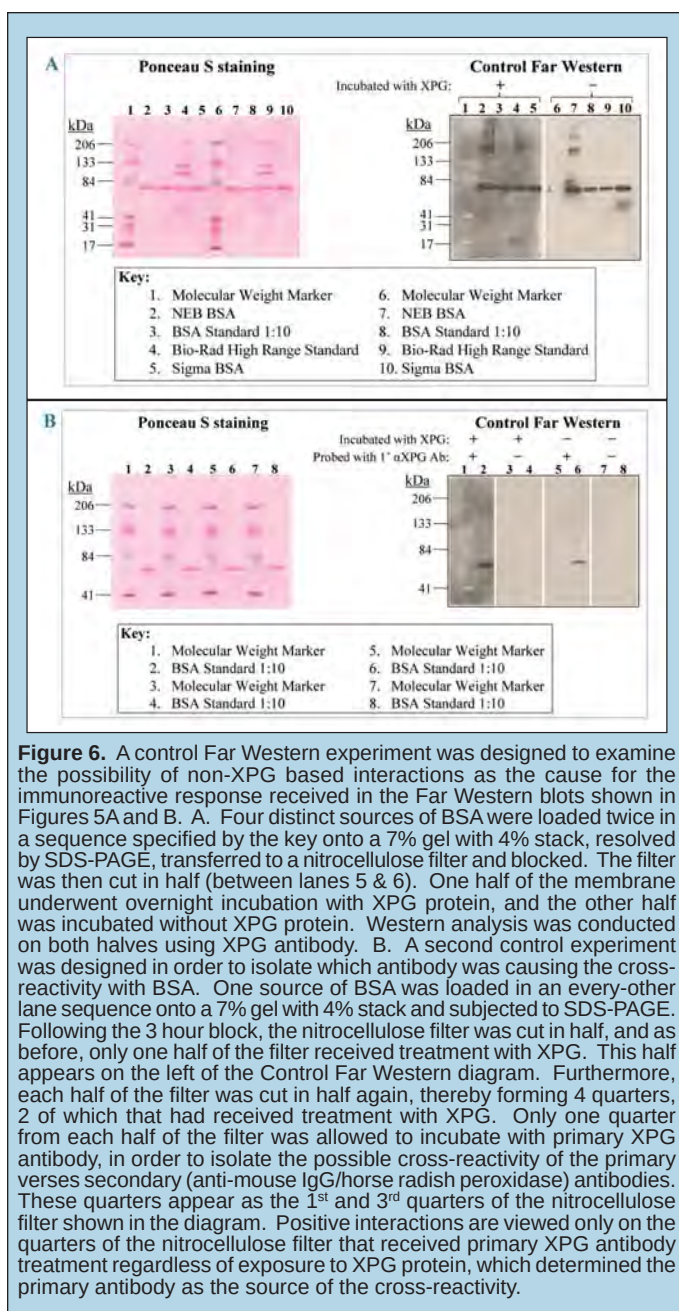
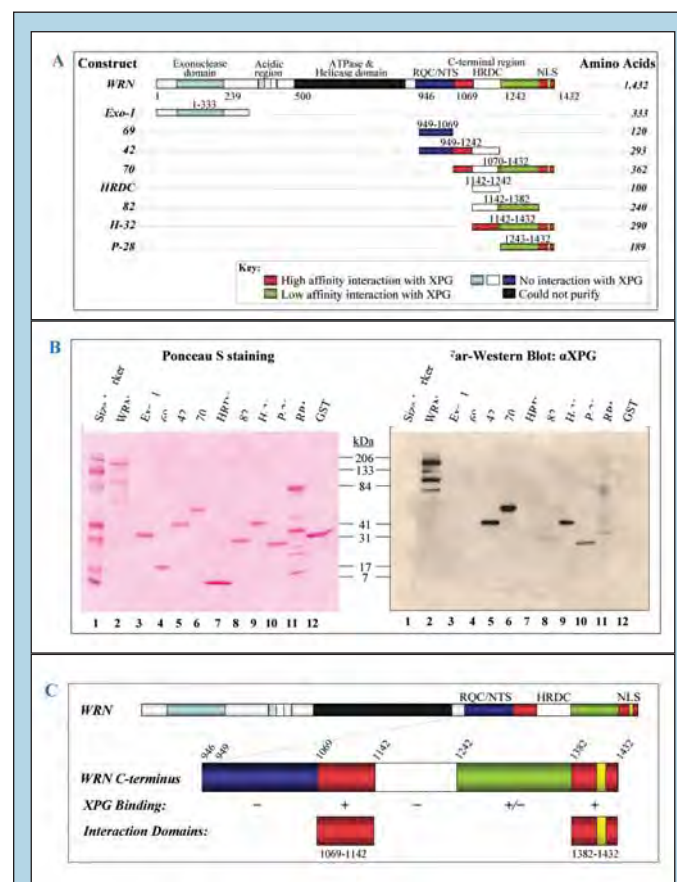


Figure 5. A) Designations for full length WRN, constructs Exo-1 and H-32 along with five control proteins that were resolved by 4–12% Tris-glycine SDS-PAGE are provided by the key. XPG was run on the gel itself in lane one to verify the efficiency of the Western detection using XPG antibody; definitive interactions should show between a protein and its antibody. Shown *left* is the Ponceau S staining of the nitrocellulose and to its *right*, protein-protein interaction bands are viewed between XPG and WRN, H-32, the positive control proteins XPG, CSB, and RPA, but also the negative control protein BSA (lane 6) after Western detection. These results are confounded by the interaction band with BSA that suggests a non-specific interaction due to error in the methodology. B) Shown are the Ponceau S staining and the anti-XPG blots of the subsequent Far Western analysis that was performed in similar fashion as 5A, with the same proteins, except two additional sources of BSA. Designations for the proteins are again provided by the key. The Far-Western blot shown on the *right*, replicates the results produced in the preliminary analysis even among the two new negative control sources of BSA (lanes 9 and 10), prompting further investigation as to the basis of reactivity for BSA.



domain deletion constructs for finer interaction mapping of this region (Figure 7A). Thus far, most of the WRN-interacting proteins have been shown to bind to more than one region within WRN protein, thus the eight total recombinant truncated WRN proteins used in the Far Western assay enabled precise mapping of the XPG binding domains of WRN (Figure 7A) [21], [22]. The inability to produce a soluble and purified helicase domain construct precludes the ability to test this region. The WRN C-terminal deletion constructs enable isolation of the RQC (aa 949-1069; construct 69), the HRDC (1142-1242; construct HRDC), and the nuclear localization signal (NLS) (aa 1243-1432; construct P-28) domains, as well as all the regions between these complexes (constructs 42, 70, 82, and H-32). Subtractive analysis can be used to identify two independent interaction domains for XPG in the WRN protein, based on the results of the Far Western assay (Figure 7B).

The interactions among the three WRN C-terminal truncation constructs 69, 42, and HRDC together isolate one of the domains of interaction. Constructs 69 and HRDC do not possess immunoreactive bands, thereby eliminating these domains as being interactive with XPG. However, a strong interaction appears for 42, a deletion construct that essentially bridges the 73 residues that separate constructs 69 and HRDC, inclusive of these regions. Thus, an independently interacting region within the WRN C-terminus



was found to reside between the RQC and HRDC domains, which comprises amino acids 1069–1142 (Figure 7C).

Additional XPG interactions with deletion constructs 82, H-32 and P-28 support the existence of a second binding site for XPG within the C-terminus. Protein construct 82 harbors a complete HRDC complex plus the next 140 of the remaining 190 5' C-terminal residues (aa 1142–1382), and displays a very weak interaction band. However, the H-32 fraction maps essentially the same region within the C-terminus as 82, in addition to the final 50 C-terminal residues (aa 1142–1432), and displays a much stronger interaction with XPG. This result suggests that the final 50 residues or amino acids 1382–1432 comprise the majority of a second XPG binding domain within the WRN C-terminus (Figure 7C). A strongly interacting P-28 construct, which maps the C-terminal region 5' to the HRDC complex, confirms this result. The weak interaction with 82 indicates that the second XPG binding domain may begin prior to the final 50 residues of WRN. Additionally, the relatively weaker interaction of XPG to P-28 as compared to H-32 could be due to ineffective folding of the shorter form which excludes the HRDC domain, thereby compromising XPG binding ability. This suggests that an intact HRDC domain may increase the WRN C-terminal ability to assume the native conformation viewed in the full length protein. The largest deletion construct of the WRN C-terminus, 70 (aa 1070–1432), which includes both interaction sites confirms these results by demonstrating the strongest immunoreactive band on the blot. Hence, WRN possesses two independent XPG interacting regions within the C-terminus.

CONCLUSION

These studies identify for the first time the C-terminal domain as the key region of XPG that is necessary and sufficient for a physical interaction with WRN, as well as two independent interaction sites of WRN that complement this interface. The fact that WRN preferentially unwinds secondarily structured DNA substrates, which are functional intermediates of the HRR subpathway of DSB repair, and that WRN is responsible for the recruitment of other proteins that mediate DNA repair in order to optimize DSB repair, provides the possibility of a novel replication-associated role for XPG within this repair pathway (Figure 8). This proposed role is supported by interactions of XPG with proteins Rad 51, BLM and

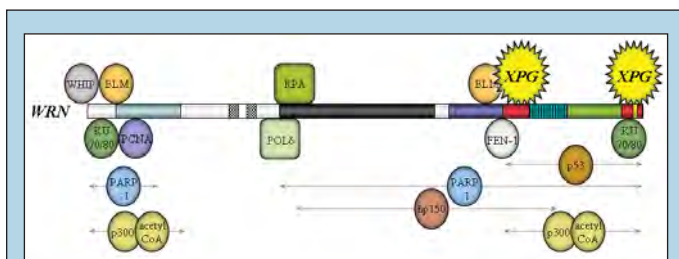


Figure 8. Select documented protein binding partners for WRN and novel interacting domains with XPG. WRN domains are again designated by the same colors used in Figure 4. Protein binding partners indicated by rectangular symbols interact with WRN, though the precise location of the interaction domain within the helicase has not been identified. Binding proteins indicated by round symbols are positioned at approximate, identified binding sites (additional binding sites may exist). Horizontal arrows indicate the limits of binding domains where the site of interaction is broad ranging or mapped less accurately. XPG is shown at its novel binding domains within the WRN C-terminus based on the results of this study.

the MRN protein complex that are also involved in the processing of stalled or collapsed DNA replication forks within HRR. The stable interaction between XPG and WRN links the repair of UV-induced DNA damage (NER), which has been made evident by the disease XP, with DSBRR, which imparts additional knowledge of the overlapping nature of these two proteins and the previously distinct repair pathways they are associated with.

The direct interaction, *in vitro*, of the XPG C-terminus with WRN is particularly interesting, given that novel structural roles of XPG in BER are mediated by this same region. Therefore, future research will focus on finely defining the interaction motifs of the XPG C-terminus with WRN protein, as well as with all other proteins identified as C-terminal binding. This investigation will involve sub-cloning and expressing three sequential MBP fused C-terminal sub-domains through polymerase chain reaction (PCR). Far Western analysis will be used to determine whether the numerous proteins that interact with XPG utilize the same region of its C-terminus or whether the interactions are mutually exclusive.

Further understanding the protein structure of the C-terminal region of XPG is additionally important due to the regions numerous interactions with BER proteins, and its likely role in CS. However, the domain has been difficult to study due to its extended and flexible conformation (Cooper Lab, unpublished results). Future studies will attempt to determine the protein structure of the C-terminal domain of XPG by forming a complex between Exon-15 (XPG C-terminus) and the smallest interacting domain of WRN that includes both regions of interaction (construct 70), in order to form a rigid structure capable of study. Initial analysis will involve using multi-angle light scattering (MALS) to determine if the XPG C-terminal extended structure has change conformation following incubation with construct 70, based upon the relative radius of the complex in solution. The precise protein structure in solution will then be determined using small angle X-ray scattering (SAXS).

The Far Western technique used in this study enabled the direct *in vitro* mapping of interaction sites between DNA repair proteins XPG and WRN that extend our understanding of these proteins' involvement in vital DNA damage repair pathways. The novel physical interaction of XPG with WRN suggests that WRN protein might be important in coordinating the possible replication-associated function of XPG at stalled or collapsed replication forks with ds breaks. Since genomic integrity is constantly threatened by both endogenous and exogenous damage, understanding the roles of these proteins in coordinating DNA repair processes with replication will significantly further understanding how their defection instigates physiological consequences in response to various DNA damaging sources. By piecing together the processes of these multifunctional proteins that restore and maintain genomic integrity, we are brought closer to understanding and preventing cancer and premature aging.

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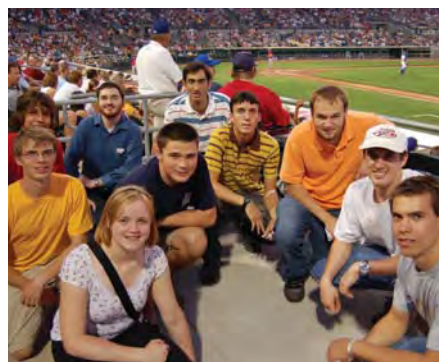
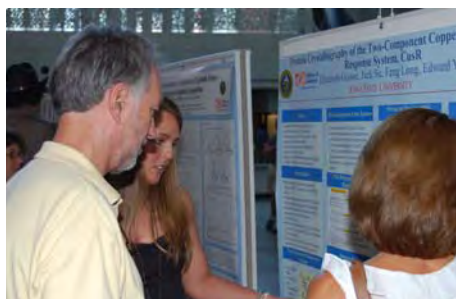
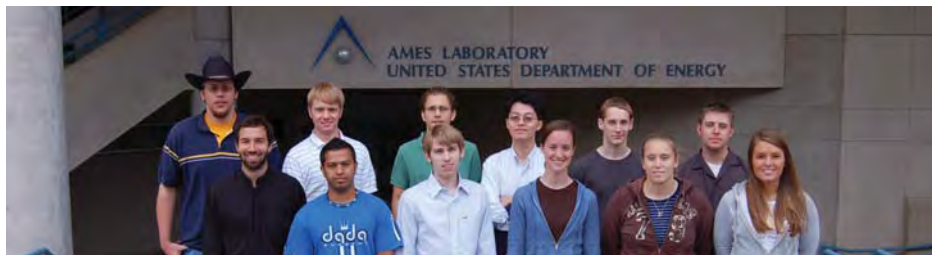
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AMES LABORATORY AMES, IOWA



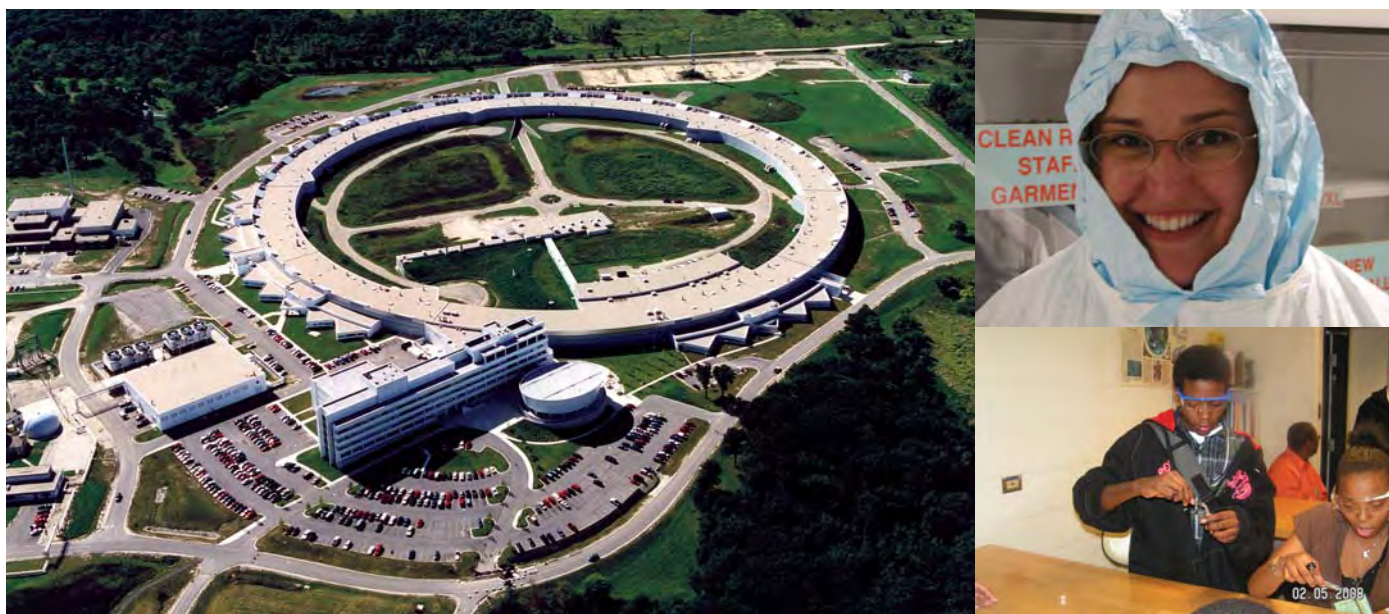
Scientists at the Department of Energy Office of Science's Ames Laboratory seek solutions to energy-related problems through the exploration of chemical, engineering, materials and mathematical sciences, and physics.

Established in the 1940s with the successful development of the most efficient process to produce high-purity uranium metal for atomic energy, Ames Lab now pursues much broader priorities than the materials research that has given the Lab international credibility.

Responding to issues of national concern, Lab scientists are actively involved in innovative research, science education programs, the development of applied technologies, and the quick transfer of such technologies to industry. Uniquely integrated within a university environment, the Lab stimulates creative thought and encourages scientific discovery, providing solutions to complex problems and educating tomorrow's scientific talent.

Ames Laboratory is located in Ames, Iowa, on the campus of Iowa State University. Iowa State's 2000-acre, park-like campus is home to more than 25000 students. Ames is approximately 30 minutes north of Des Moines, Iowa's capital city.

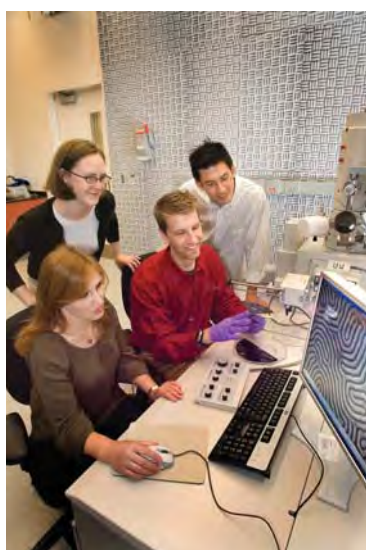
ARGONNE NATIONAL LABORATORY ARGONNE, ILLINOIS



The University of Chicago's Metallurgical Laboratory, part of the World War II Manhattan Project, gave rise to Argonne National Laboratory. The laboratory has about 2 900 employees, including about 1 000 scientists and engineers. Argonne occupies 1 500 wooded acres in DuPage County, Illinois, about 25 miles southwest of Chicago's Loop. Argonne research activities fall into broad categories:

- **Basic Science:** Basic science seeks solutions to a wide variety of scientific challenges. This includes experimental and theoretical work in materials science, physics, chemistry, biology, high-energy physics, and mathematics and computer science, including high-performance computing. This kind of basic research brings value to society today by helping lay the foundation for tomorrow's technological breakthroughs.
- **Facilities:** Scientific facilities like Argonne's Advanced Photon Source help advance America's scientific leadership and prepare the nation for the future. The laboratory designs, builds and operates sophisticated research facilities that would be too expensive for a single company or university to build and operate. They are used by scientists and engineers from Argonne, industry, academia and other national laboratories, and often by researchers from other nations. The laboratory is also home to the Argonne Tandem Linear Accelerator System, the Center for Nanoscale Materials, the Argonne Leadership Computing Facility and other facilities.
- **Energy Programs:** Energy resources programs help insure a reliable supply of efficient and clean energy for the future. Argonne scientists and engineers are developing advanced technologies and systems for a number of energy applications, including nuclear reactors, batteries and fuel cells, transportation, and electric power generation and storage programs.
- **Environmental Management:** Environmental management includes work on managing and solving the nation's environmental problems and promoting environmental stewardship. Research in this area includes alternative energy systems; environmental risk and economic impact assessments; hazardous waste site analysis and remediation planning; electrometallurgical treatment to prepare spent nuclear fuel for disposal; and new technologies for decontaminating and decommissioning aging nuclear reactors.
- **National Security:** National Security has increased in significance in recent years for the nation and for Argonne research. Argonne capabilities developed over the years for other purposes are helping counter the threats of terrorism. These capabilities include expertise in the nuclear fuel cycle, biology, chemistry, and systems analysis and modeling. This research is helping develop highly sensitive instruments and technologies to detect chemical, biological and radioactive threats and identify their sources. Other research is helping to detect and deter possible weapons proliferation or actual attacks.
- **Workforce Development:** Argonne's Division of Educational Programs provides workforce development to benefit researchers from postdocs, university faculty and students to regional K–12 schools.

BROOKHAVEN NATIONAL LABORATORY UPTON, NEW YORK

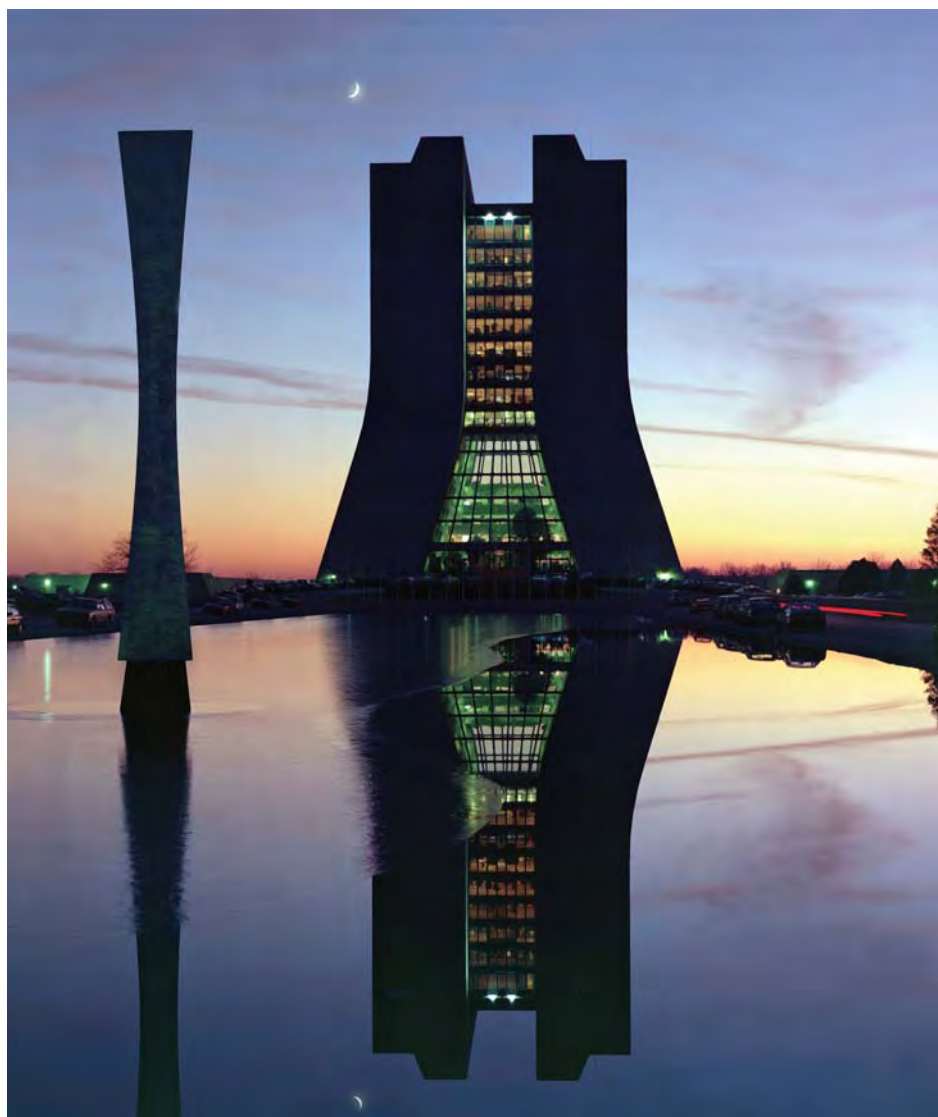


Brookhaven National Laboratory is a Department of Energy, Office of Science multidisciplinary laboratory managed by Brookhaven Science Associates, a company founded by Battelle and Stony Brook University. Home to six Nobel Prizes, Brookhaven conducts research in the physical, biomedical, and environmental sciences, as well as in energy technologies and national security.

Located on a 5300-acre site on eastern Long Island, New York, Brookhaven builds and operates major scientific facilities available to university, industry and government researchers. Among these facilities are the Relativistic Heavy Ion Collider, where physicists study the nature of matter as it existed at the beginning of the universe; the National Synchrotron Light Source (NSLS), where researchers use beams of x-ray, infrared and ultraviolet light to study materials as diverse as computer chips and proteins; and the Laboratory's newest facility, (pictured here) the Center for Functional Nanomaterials (CFN). Scientists at the CFN study and fabricate materials on a scale of a billionth of a meter. These materials can possess different chemical and physical properties than their larger-scale counterparts. The research at the CFN is focused on developing clean and efficient forms of alternative energy to replace fossil fuels.

In addition, the NASA Space Radiation Laboratory, where scientists study the effects of space radiation on astronauts, is based at Brookhaven, and the Laboratory is home to one of the fastest supercomputers in the world, New York Blue. In 2009, Brookhaven will begin construction of a new synchrotron, the NSLS-II. When it becomes operational in 2015, it will be the world's brightest synchrotron, which will enable research advances in numerous fields.

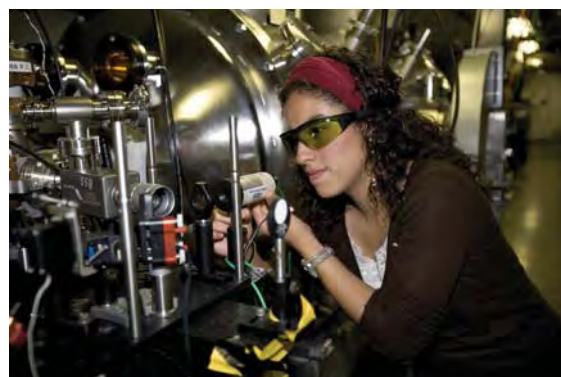
FERMI NATIONAL ACCELERATOR LABORATORY BATAVIA, ILLINOIS



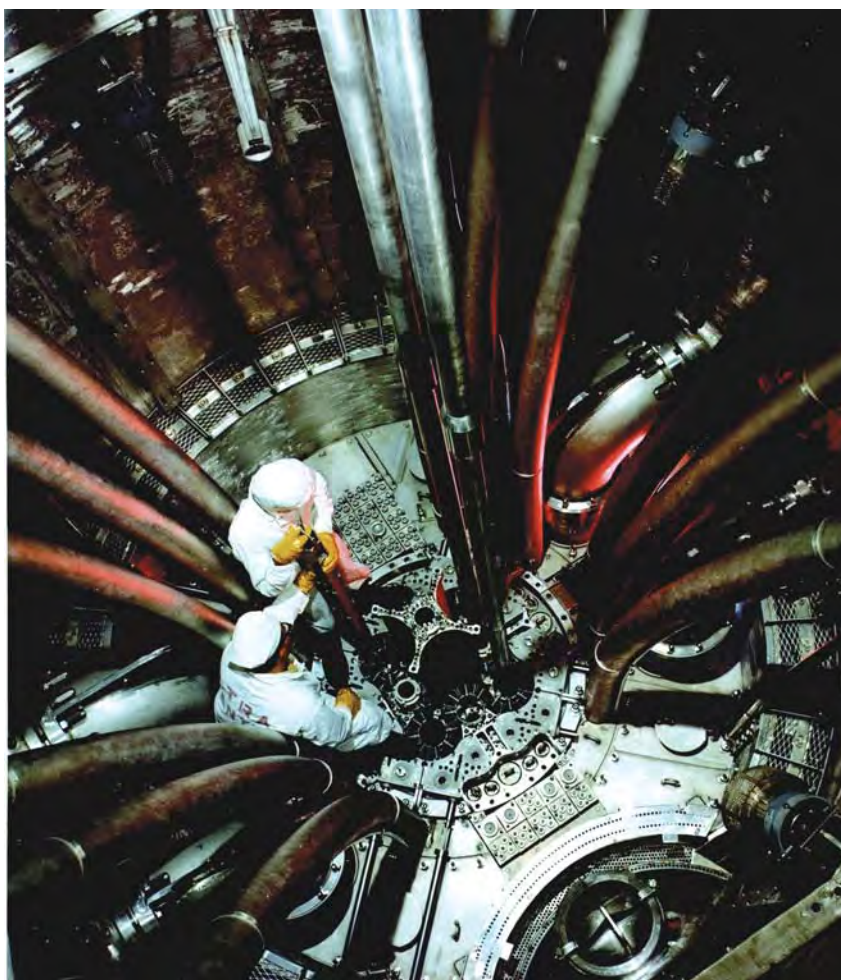
Fermi National Accelerator Laboratory (Fermilab) is one of the world's foremost laboratories dedicated to high-energy physics research. It is operated for the Department of Energy Office of Science by a consortium of 90 research-oriented universities. More than 3000 scientists from around the world use Fermilab for their experiments.

Fermilab is located on a 6800-acre site about 35 miles west of Chicago, Illinois. The laboratory is home to the Tevatron Collider, the world's highest-energy particle accelerator. Two large detectors analyze the Tevatron's proton-antiproton collisions to unveil the fundamental forces and particles of the universe. Scientists at Fermilab discovered the bottom quark and the top quark, and first observed the tau neutrino.

Fermilab operates the world's most powerful proton beam for creating neutrinos. The Center for Particle Astrophysics at Fermilab includes groups studying cosmic rays, supernovae, dark energy and other phenomena.



IDAHO NATIONAL LABORATORY IDAHO FALLS, IDAHO



In operation since 1949, The Idaho National Laboratory (INL) is a science-based, applied engineering National Laboratory dedicated to supporting the U.S. Department of Energy's missions in nuclear and energy research, science, and national defense.

INL stands out as a unique national and international resource. Notably, the Lab has been formally designated as the nation's command center for advanced civilian nuclear technology research and development, and is home to the unparalleled Critical Infrastructure Test Range, with assets as diverse as an isolable electric grid and wireless test bed. Leveraging these and numerous other distinguishing features, the Lab and its more than 3300 scientists, engineers and support personnel build on the potential and promise of the theoretical for the benefit of the real world.

Located in southeast Idaho, INL covers 890 square miles of the Snake River Plain between Idaho Falls and Arco, Idaho. Offices and laboratories are also in the city of Idaho Falls (population 50 000), located about two hours from Grand Teton and Yellowstone national parks and other areas offering prime recreational opportunities.



LAWRENCE BERKELEY NATIONAL LABORATORY BERKELEY, CALIFORNIA



Lawrence Berkeley National Laboratory's (LBNL) research and development includes new energy technologies and environmental solutions with a focus on energy efficiency, electric reliability, carbon management and global climate change, biofuels, and fusion. Frontier research experiences exist in nanoscience, genomics and cancer research, advanced computing, and observing matter and energy at the most fundamental level in the universe.

Ernest Orlando Lawrence founded the Berkeley Laboratory in 1931. Lawrence is most commonly known for his invention of the cyclotron, which led to a Golden Age of particle physics — the foundation of modern nuclear science — and revolutionary discoveries about the nature of the universe. Berkeley Laboratory has several premier national user facilities, such as the Molecular Foundry, the National Center for Electron Microscopy, and the Advanced Light Source, centrally located on the Laboratory site overlooking the San Francisco Bay.



LAWRENCE LIVERMORE NATIONAL LABORATORY LIVERMORE, CALIFORNIA



Lawrence Livermore National Laboratory (LLNL) applies cutting-edge science and engineering to enhance the nation's security. When LLNL was founded in 1952, the consuming national security concern was the nuclear arsenal of the Soviet Union and, for years, our energies, talents and resources were focused on that threat. Today, new perils have arisen that are radically different and vastly more complex, and we are directing our world-class scientific and technological resources against these threats. Assuring the safety, security, and reliability of the nation's nuclear weapon stockpile continues to be the foremost responsibility of LLNL. We are also pushing the frontiers of science and technology to make breakthroughs that will be able us to meet future needs in national and global security, energy and environment, and economic competitiveness.

LLNL is home to some of the world's most powerful supercomputers, including BlueGene/L, first on the TOP500 list of supercomputers with a sustained world-record speed of 478.2 teraflops. LLNL also supports unique experimental facilities, including the Center for Accelerator Mass Spectrometry, the High Explosives Applications Facility, and the 192-beam National Ignition Facility, which is the world's largest laser system. Our researchers typically work in multi-disciplinary teams, where experts in physical and life sciences, engineering, and computations collaborate to devise and demonstrate solutions to nationally important problems.

LLNL offers numerous opportunities for outstanding scholars and postdoctoral fellows to complement their academic endeavors and enable them to work on exciting areas of research using our advanced experimental facilities and computing resources. Laboratory scientists, many of whom are leading experts in their fields, guide and collaborate with student researchers and have earned numerous commendations as outstanding mentors.

On the local level, the Laboratory offers a wide array of student science enrichment and teacher development programs tied to LLNL science and technology that benefit more than 25000 K-12 students and teachers each year. Programs include college-accredited teacher research academies and research internships, community science lectures, a science and engineering project competition, tours for school groups, and special educational outreach events.

LLNL is located on a mile-square site at the eastern edge of the Livermore Valley, roughly an hour from San Francisco, two hours from the Pacific Ocean, and three hours from the Sierra Nevada mountains. The Laboratory is managed for the Department of Energy's National Nuclear Security Administration by Lawrence Livermore National Security LLC, a consortium of Bechtel National, University of California, Babcock & Wilcox, Washington Division of URS Corporation, and Battelle.

LOS ALAMOS NATIONAL LABORATORY LOS ALAMOS, NEW MEXICO



The Los Alamos National Laboratory (LANL), located in the Jemez Mountains of northern New Mexico, offers the opportunity for students to work at a multi-disciplinary, world-class research facility while enjoying a truly unique environment. Long known for its artistic community, northern New Mexico also offers a variety of exciting outdoor recreational opportunities, including rock climbing and hiking in the adjacent mountains and canyons, proximity to the Rocky Mountains, and exceptional skiing opportunities at many nearby locations.

We offer a diverse research experience for undergraduate and graduate students as a means of assuring the continued vibrancy of the science, engineering, and technology at the laboratory. Serve your internship with us and you will have the opportunity to work in a team environment with some of the world's top scientists and engineers on critical issues involving our national security, environment, infrastructure, and security. We offer internship opportunities in areas that include: Biology, Chemistry, Computer Science, Physics, Mathematics, Materials Science, Environmental Science, and Engineering: Chemical, Civil, Computer, Electrical, Mechanical, Nuclear, and Software.

If you are a problem solver and independent thinker, a team player, a good communicator, like a hands-on approach, and are self-motivated, we offer you the challenge of an internship at LANL.

NATIONAL RENEWABLE ENERGY LABORATORY GOLDEN, COLORADO



The National Renewable Energy Laboratory (NREL) is the U.S. Department of Energy's primary National Laboratory for renewable energy and energy efficiency research and development. From harvesting energy from the sun and wind, to advancing automotive systems, to developing biodegradable plastics from corn stalks, NREL develops renewable energy and energy efficiency technologies and practices, advances related science and engineering, and transfers research knowledge and innovations to address the nation's energy and environmental goals. NREL takes its research to the community through projects such as building Zero Energy Habitat for Humanity Homes, education outreach, teacher workshops and sponsoring interns.

NREL research has been recognized with 44 R&D Awards, ranking first among National Laboratories per researcher, as well as numerous honors from R&D, Discover, and Popular Science magazines and leading scientific organizations. Scientist mentors work with over 200 interns annually in developing the future workforce.

Innovative, challenging and dynamic — that's our culture. If you are interested in a research internship with an institution that believes creativity and individual uniqueness is at the core of our success, then explore your options at: www.nrel.gov. We value intern talent that adds to the rich pool of research findings produced by NREL each year. Intern accomplishments include:

- More than 27 students have been selected by the Office of Science to present major NREL research at the AAAS.
- More than 50 past student interns have been hired at NREL.
- Teacher researchers have produced over 50 renewable energy lessons for the classroom.
- Two student/scientist patents have evolved from internships.
- NREL's Education Program partners with over 40 universities throughout the nation.

NREL's main 327-acre site is in Golden, Colorado, just west of Denver. The Laboratory also operates the National Wind Technology Center on 307 acres about 20 miles north of Golden. We are an equal opportunity employer committed to diversity.

OAK RIDGE NATIONAL LABORATORY OAK RIDGE, TENNESSEE



Oak Ridge National Laboratory (ORNL) is the U.S. Department of Energy's (DOE) largest science and energy laboratory. Managed since April 2000 by a partnership of the University of Tennessee and Battelle, ORNL was established in 1943 as part of the secret Manhattan Project to pioneer a method for producing and separating plutonium. Today ORNL has a research portfolio in excess of \$1.3 billion, a staff of more than 4 200 and approximately 3 000 guest researchers (undergraduates, graduate students, postgraduates, teachers, and faculty) who spend two weeks or longer each year in Oak Ridge. The \$1.4 billion Spallation Neutron Source, located adjacent to the new Center for Nanophase Materials Sciences, and the High Flux Isotope Reactor are rapidly making Oak Ridge one of the world's foremost locations for the study of materials. ORNL's National Leadership Computing Facility now houses the world's most powerful open science supercomputer and soon will house a computer capable of a mind-boggling 1 000 trillion calculations per second. Each of these facilities will work closely with ORNL's new Bioenergy Science Center, funded by DOE to develop breakthrough technologies for cellulosic ethanol.

Since 2000, UT-Battelle has provided more than \$8.25 million in support of math and science education, economic development, and corporate volunteerism in the greater Oak Ridge region as well as various civic, cultural and public awareness activities related to DOE's mission.



PACIFIC NORTHWEST NATIONAL LABORATORY RICHLAND, WASHINGTON



Pacific Northwest National Laboratory (PNNL), on the sunny eastern side of Washington State, is one of the U.S. Department of Energy's (DOE) ten national laboratories, managed by DOE's Office of Science. PNNL has been proudly operated by Battelle since 1965 and performs research for other DOE offices as well as government agencies, universities, and industry to deliver breakthrough science and technology to meet today's national needs. PNNL is home to the William R. Wiley Environmental Molecular Sciences Laboratory, a DOE Office of Science national science user facility. On the campus of Washington State University (WSU) Tri-Cities in Richland, Washington, researchers from WSU and PNNL collaborate in the new Bioproducts, Sciences, and Engineering Laboratory to convert biomass into value-added fuels and chemicals. PNNL also operates the Sequim Marine Research facility in western Washington.

National security, energy demands, and environmental impacts are some of America's toughest challenges. At PNNL, we are driven to provide science and solutions to meet these challenges. We accomplish this mission through the power of our interdisciplinary teams, bringing together experts from multiple disciplines to tackle complex problems.

Through fundamental research, we generate new knowledge, new understanding, and transformational tools and techniques. These new insights and tools are advancing scientific frontiers in the molecular, environmental, biological, and computational sciences. Collaborating with our partners, PNNL is developing ways to use today's energy sources more cleanly and efficiently while helping shift our nation to more renewable resources. As national security threats become more complex and unpredictable, our technologies are becoming more sophisticated to keep pace. Our tools and methods are helping others prevent and counter terrorism and the proliferation of weapons of mass destruction. Environmental innovations from PNNL are being used to protect water sources, clean up underground contamination, and explore how greenhouse gases can be stored in deep geologic formations.

We champion science, technology, engineering, and mathematics (STEM) education from "grade school to grad school" in order to support the "college and workforce ready" agenda of the nation, DOE, our region, and local communities. We help to develop and educate the scientists and engineers of the tomorrow. We strive to impact STEM education by acting as a catalyst for sustainable positive change on national, regional, and local levels. This includes providing thought leadership, creating business-in-education partnerships, participating in scalable initiatives, and advancing the progress of existing programs that have proven results, but require additional resources and partnerships to broaden their impact.

PRINCETON PLASMA PHYSICS LABORATORY PRINCETON, NEW JERSEY



The world's reliance on fossil fuels is imperiling our environment. Fusion, the energy source of the sun and the stars, offers an inexhaustible alternative. A fusion-powered electric generator would not produce hydrocarbon emissions, greenhouse gases, or long-lived radioactive waste; nor would it emit chemicals that cause acid rain. Consequently, the U.S. Department of Energy (DOE) Office of Science has made the development of commercial fusion power one of its highest priorities.

DOE's Princeton Plasma Physics Laboratory (PPPL) is one of the world's leading facilities for fusion R&D. Currently PPPL is operating the National Spherical Torus Experiment, which uses magnetic fields to confine hot ionized gas (plasma) that serves as the fusion fuel. PPPL's theoretical physicists are developing computational physics models that can predict how various plasma configurations will perform, saving time and money.

PPPL experimental physicists collaborate with their colleagues worldwide in a free, mutually beneficial, exchange of information. Princeton researchers and engineers use knowledge and skills gained in fusion research to solve other problems, including the development of plasma-based propulsion systems for space vehicles, studies of plasma phenomena that occur in the sun's corona and the earth's magnetosphere, and nuclear detection systems.

The Laboratory interacts with the nearby community through its tour program, Speakers' Bureau, and Science Education Program (SEP). The goal of the PPPL SEP is to combine the core research activities of PPPL with science education programs to create a center of excellence for students and teachers. To achieve its goals, the SEP strives to: (1) contribute to the training of the next generation of scientists and engineers, (2) collaborate with K-12 teachers on ways to improve science teaching using an inquiry-based approach to learning, and (3) improve the scientific literacy of the community at large. These initiatives, led by SEP staff in conjunction with PPPL volunteers, master teachers, and local education experts, create significant learning opportunities for undergraduate college students and K-12 teachers and students. PPPL is about three miles from Princeton University's main campus in Princeton, N.J.

SLAC NATIONAL ACCELERATOR LABORATORY MENLO PARK, CALIFORNIA



SLAC National Accelerator Laboratory is one of the world's leading laboratories for research in photon science, astrophysics, and accelerator and particle physics.

The laboratory's programs explore the structure and dynamics of matter as well as the properties of energy, space and time — at the smallest and largest scales, in the fastest processes and at the highest energies. Through SLAC's investigations into how matter behaves on multiple time, length and energy scales, researchers address major scientific and technological challenges affecting society at large.

By delving into the smallest scale of matter, SLAC scientists answer fundamental questions about the most basic constituents of matter and the forces between them; create materials with extreme strength, flexibility and heat resistance; seek cleaner, greener technologies; and gain better control of molecules on the nanoscale.

Laboratory researchers also study matter on the largest scale, looking to the skies and conducting experiments deep underground to explore the history and evolution of the universe, reveal the mysteries of cosmic objects and search for new fundamental laws of nature.

SLAC is located on the Stanford University campus in Menlo Park, California. Six scientists have been awarded the Nobel Prize for work carried out at SLAC, and the future of the laboratory promises to be just as extraordinary.

THOMAS JEFFERSON NATIONAL ACCELERATOR FACILITY NEWPORT NEWS, VIRGINIA



The Thomas Jefferson National Acceleration Facility, or Jefferson Lab, is a nuclear physics research laboratory located in Newport News, Virginia. Nuclear physics research scientists who use Jefferson Lab are on a journey of discovery into the nucleus of the atom. Their goal is to develop a roadmap of matter that helps unlock the secrets of how the universe is put together. Nuclear physics funding from the Department of Energy provides Jefferson Lab with leading-edge instrumentation, world-class facilities and training and support for the people involved in these pursuits. Forefront nuclear physics research conducted at Jefferson Lab provides solid foundations for other fields. The accumulation of new results and the intellectual training of new generations of scientists foster important advances in medicine, chemistry and other sciences.

Scientists at Jefferson Lab use the Continuous Electron Beam Accelerator Facility — the first large-scale application of superconducting radiofrequency technology — to conduct physics experiments. Using accelerated electron beams, experimenters probe the sub-nuclear realm. Using this same technology, Jefferson Lab has built the world's brightest high average power Free Electron Laser that offers unique capabilities for defense, industry, basic research and medicine.

NATIONAL SCIENCE FOUNDATION, A VALUED PARTNER

The National Science Foundation (NSF) supports collaborative projects involving academic institutions, private industry and state and local governments. The Foundation works closely with the U.S. Department of Energy in cross-cutting areas of research and education, including sharing in the costs of sponsoring undergraduate intern placements at the National Laboratories. Collaboration and partnerships between disciplines and institutions and among academe, industry and government enable the movement of people, ideas and tools throughout the public and private sectors.



An asterisk by the abstract title in this journal indicates students whose work is funded in part by NSF.



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Many participants in the DOE's undergraduate research programs are supported by grants from the National Science Foundation. These participants are designated with an "*" preceding the title of their abstract.

Biology

Analysis of Subsurface Microbial Communities from the Hanford 300 Area

Nicholas Adams (MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY, ROLLA, MO 65401), Allan Konopka (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352).

Microbial communities that encompass the Hanford 300 area as well as their respective ecological niches have been rarely, if at all, observed and analyzed. The Hanford 300 area is somewhat unique to the Washington area, in that it has been classified as a semi-arid area located parallel to a major river (Columbia). It also has the unique property of being located within the bounds of a retired complex of uranium/plutonium production plants. This presents the opportunity to study the relationship between bacterial communities in their native environment and an abundance of potentially radioactive elemental byproducts of the 300 Hanford area. Microbial communities in subsurface soil samples, collected from various wells and geological strata, were investigated from the surface down to a depth of 61 feet in the shallow bore-holes and down to 172 feet in the microbiological deep-borehole. Gradient tubes, dilution to extinction, as well as most probable number (MPN) plates were prepared using varying terminal electron acceptors such as iron oxide, manganese oxide, sodium sulfate and sodium nitrate. These two tests were also developed using low amounts of carbon substrate to mimic that of soil content. Preliminary findings based on liquid media and gradient tube growth suggest that there are a number of microorganisms with the capability of reducing not only manganese oxide and iron, but also certain sulfate and nitrate groups as well. These early findings suggest the possibility of remediation-capable microorganisms that are already in the area of radioactive contamination.

Comparative Study of the Beclin 1 and LC3 Markers in the Autophagic Process

Nabras Ahmed (HONORS COLLEGE AT STATE UNIVERSITY OF NEW YORK—STONY BROOK, STONY BROOK, NY 11790), Qiong Liu (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

Autophagy is a catabolic process by which a cell degrades its own components using its lysosomal digestive mechanism. This process takes place when double-membrane bound components, called autophagosomes, transfer materials from the cytoplasm to the lysosome(s). The microtubule-associated protein 1 light chain 3 (LC3) protein is a well accepted marker for autophagy because it binds to the autophagosome membrane. Another marker used to evaluate autophagy is the gene Beclin 1. Beclin 1 has been found to participate in the formation of autophagosomes and thus is considered a marker to identify autophagic activity. However, it is not clear if these two markers behave similarly in cultured cells. The experiment here intends to understand the differences between the LC3 and Beclin 1 marker in order to better understand what roles they play in the autophagic process. We will starve cultured HEK 293T cells for different periods of time to induce the autophagy process, and we will count the cells that were labeled by EGFP-LC3 and EGFP-Beclin1, differently. We are still in the experimental stage of this study and have yet to reach any conclusions.

Expression of Stem Cell Markers in Individual Cells Across a Colony Using Duplex RT-PCR

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Although stem cells may appear to be identical, more evidence from recent studies demonstrate they are heterogeneous within a colony. Each cell in the colony may have a different expression level depending on its different local environment in the colony. The expression of stem cell markers is commonly detected for entire stem cell colonies. The goal of this project is to conduct gene analysis against an individual cell in the colony. In order to verify if a colony has an equal concentration of markers throughout the whole population, non-isolated stem cell RNA was obtained by a freeze-thaw method. Using Reverse Transcriptase Polymerase Chain Reaction (RT-PCR) in combination with molecular beacons, a procedure for the quantification of marker using fluorescence was studied. A correlation between relative fluorescence signal (RFU) and RNA concentration was investigated by attaching the site-specific molecular beacon to the corresponding DNA of the gene during the RT-PCR. Oct-4 was used as standard marker for human embryonic stem cell, and Actin, a housekeeping gene, was used as a control. The Oct-4 gene gave a satisfactory correlation with increasing stem cell concentration. However, further optimization is necessary for single cell expression detection. Initially, the Actin probe did not show any correlation with respect to stem cell concentration. Later, the

probe was modified and gave preliminary good results but needs more repetition to prove its consistency.

Fatty Acid Profile in *Prunella vulgaris*

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Prunella vulgaris is a herbaceous plant in the family *Lamiaceae*, also known as 'heal all'. *P. vulgaris* is commonly used in folk medicine for the treatment of herpes, skin diseases, food poisoning, blood pressure, inflammations, etc. My objective is to study the Fatty acid (FA) profile in *P. vulgaris*. Fresh plant tissue was collected from USDAARS-North Central Regional Plant Introduction Station in liquid nitrogen. Then the samples were grounded and lyophilized. Fatty Acid was extracted using the Barium Hydroxide Hydrolysis method. The extracted sample was run through the Gas Chromatograph Mass Spectrometer (GC-MS) to analyze the chemical components. My project was focused on comparing FA in the flower and leaf of *P. vulgaris*, *P. vulgaris* from different accessions (27666-Ohio, 27664-North Carolina and 27648-Missouri) and in two-year and three-year old plants. After the complete study, it was found that the common fatty acids present in the plant were Palmitic Acid, Steric Acid, oleic Acid, Linoleic Acid, A-linolenic Acid and lead Lonophore V. Among them, Palmitic Acid and Linoleic Acid is found more in flowers than in leaves, while others are fairly in same ratio. Results of our study also showed that there is no significant difference of FA profile in plants of different accessions and two-year and three-year old plants.

Expression of a Heat-Tolerant Cellulose Digesting Enzyme in *Escherichia coli*

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Fuel ethanol is currently made from plant-derived sugars. The development of renewable biofuels capable of displacing current fossil fuels will require significant innovation and improvement. These second generation biofuels are not derived from grain or food, but are instead derived from feedstocks such as corn stover or agricultural waste, according to Dr. Andersen & Lawrence Berkeley National Laboratory in 2007. One critical step in the conversion of second-generation biofuels from lignocellulosic biomass is the depolymerization of polysaccharides, such as cellulose, into the respective monosaccharides, such as glucose. To be industrially useful, the breakdown process must be stable at high temperatures that enable consolidated bioprocessing. A gene for an enzyme that breaks down cellulose at high temperatures was isolated from the high temperature-tolerant bacterium, *Acidothermus cellulolyticus*, and the gene was placed in a circular DNA structure called a plasmid. This plasmid had a promoter, that caused elevated expression level of messenger RNA which caused the production of large amounts of the cellulose-digesting enzyme. The plasmid was placed in a particular non-pathogenic strain of bacteria called *Escherichia coli* BL21 DE3. The bacterium was grown in large quantities and then the enzyme was isolated from bacterial cells that had been broken open to release the enzyme. Sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), which separates molecules by size alone, showed the enzyme to be present in all samples. Three other tests for the enzyme were performed. First, a protein isolation technique, called gel electrophoresis, separated the multiple proteins from the *E. coli* and allowed the specific cellulose-digesting enzyme to be identified. Second, a flat dish containing cellulose embedded in a solidifying agent, agar, was stained with congo red. Two different samples of cellulose-digesting enzyme, one kept at room temperature and one heated for five minutes at 100 °C, in addition to the control, were placed on the red-stained agar and allowed to digest the cellulose. This produced a clear area around both samples, but not the control, and confirmed that the heated enzyme was just as active as the room temperature enzyme at these conditions. Third, the rate of digestion by room temperature and heat-treated enzyme was quantified, using carboxyl-methyl-cellulose dyed with remazolbrilliant blue (azo-CMC) and analyzed via spectrophotometry and showed that heating to 100 °C for five minutes destroyed enzyme activity. Thus the two tests, congo red and azo-CMC, (assays for heat stability of the enzyme) gave conflicting results. A discussion of these results and a probable theorem of their origin will be presented hereafter.

Effects of Cigarette Smoke Cadmium on the Release of Calcium from Bone in Humans

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During World War II, mining companies in Japan polluted the local Jinzu River with large amounts of cadmium. People living downstream, who used the polluted water for drinking and irrigation, were exposed to

high levels of cadmium for a significant amount of time. These people, particularly postmenopausal women, developed Itai-itai disease, which is characterized by kidney failure and osteomalacia, or softening of the bones. The aim of this research project is to determine whether cadmium from cigarette smoke has a similar influence, namely, contributing to osteoporosis in postmenopausal women. Cigarettes provide an external dose of cadmium that can cross from the lungs to the blood. Because postmenopausal women have a considerable decrease in estrogen levels, their bones are less protected from bone resorption. The project comprises two successive studies. Study 1 aims to characterize cadmium exposure due to cigarette smoke in postmenopausal women and age-matched men. A smoking machine was used to "smoke" the brand of cigarettes that each participant smokes and trap the cadmium-containing smoke particulates on a quartz filter. The cadmium measured for each cigarette varied from brand to brand. This suggests that participants are receiving different doses of cadmium (Cd) depending on the brand they smoke. The highest Cd measured was from unfiltered Pall Mall cigarettes. The lowest Cd measured was from True Menthols cigarettes. Samples of blood, urine and serum were collected from each participant. The data from the Cd concentration in cigarettes will be compared to the Cd concentration in the human samples once analyzed to see if there is any correlation. For Study 2, each female participant was injected with 100 nanocuries of ^{41}Ca (Calcium), which is incorporated into bones over a four month period. During Study 2, ^{41}Ca measurements will be made during a three-week baseline period in smokers and non-smokers. Smokers will then be asked to stop smoking for a period of three weeks. The change in smoking status allows us to measure the relationship between calcium release and a change in cadmium exposure (smoking cessation), using ^{41}Ca to ^{40}Ca ratio in urine to evaluate calcium release from bone. We will use the Accelerator Mass Spectrometry (AMS) facility at Purdue University to quantify the ^{41}Ca levels. The results of the study will be analyzed and documented in late 2008. Determining the extent to which cadmium in cigarette smoke affects osteoporosis will help us to understand the mechanisms of bone loss and to evaluate the impact of environmental cadmium on skeletal integrity in humans.

Characterization of Sensor Proteins from *Clostridium thermocellum*

Perry Bradford (ILLINOIS MATHEMATICS AND SCIENCE ACADEMY, AURORA, IL 60120), Frank Collart (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). Proteins are an essential part of cells that aid in transport, signal transduction and sensing the environment. Proteins that sense the environment are called sensor proteins. In microbes, these proteins bind various environmental ligands and couple this action to intracellular signals that mediate microbial response. In this study, we used a ligand binding procedure to map sugars to a group of 48 sensor proteins from *Clostridium thermocellum*. The open reading frames (ORFs or genes) were amplified via polymerase chain reaction (PCR) and then annealed into the vector. The coding region fragments were cloned into pMCSG7, a cytoplasmic expression vector with an N-terminal 6xHis fusion tag. The expression constructs were inserted in competent *Escherichia coli* BL21 cells by transformation and plated to obtain single colonies. After testing for positive expression and solubility, a total of 12 soluble proteins were chosen as our targets based on their annotation as ABC-type sugar transport or amino acid transport proteins. The 12 targets were scaled-up and purified by affinity chromatography on Ni-NTA beads. A fluorescence-based thermal shift assay was used for identification of binding ligands to the 12 targets. High-throughput screening of 12 proteins against six ligand pools identified specific binding to trehalose for a putative sugar-binding protein as well as binding to spermine for a transporter protein predicted to bind spermidine and putrescine. The results from this project will improve gene/protein functional assignments of sensor proteins and develop high-throughput methods to match ligands with their specific binding proteins.

Sequencing of Bacterial Genomes: An Emphasis on Wet Lab Techniques and Biology as an Information Science

Hilary Briggs (UNIVERSITY OF REDLANDS, REDLANDS, CA 92374), Chris Detter (LOS ALAMOS NATIONAL LABORATORY, LOS ALAMOS, NM 87545). In 2003, after three billion dollars and 13 years of international work, the sequence of the human genome was completed. Presently, with the large demand for energy, alternative ideas for waste management and the advancing ease and efficiency of sequencing, the Joint Genome Institute (JGI) is far from finished. The methodology central to genomic sequencing has changed drastically, and with the acceleration of technology will continue to do so for years to come. The original techniques functioned via breaking up the genome into many

fragments, amplifying them, and using capillary electrophoresis to phosphoresce fluorescently labeled DNA. This system uses 384 well plates, each of which holds five to eight micro liters of a sample, and is still in use today. The contemporary procedures use plates with millions of wells and pico liters of volume. It is quite easy to imagine, therefore, the vast expansion in sheer numbers of base pairs sequenced. As one gear in the vast machine of sequencing, the Los Alamos branch of the JGI and my contribution therein, have focused on the many varieties of sequencing techniques, the fundamental and innate science that enables these methods, the flow of organisms through the sequencing systems, and the abundance of information being produced by genetics. In my work I looked into the processes that are used today, the movement of a species through the JGI, and the consistent and laborious task of maintaining masses of data.

Rapid Detection of Molecular Changes Associated with Antibiotic Resistance in *Yersinia pestis*

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The advent of modern medicine, particularly antibiotic use and enforcement of public health measures, have significantly reduced the frequency and severity of plague outbreaks worldwide. However, the protection that antibiotics provide against the causative agent of plague, *Yersinia pestis*, may be short-lived. This project aims to investigate the genetic basis and molecular mechanisms underlying antibiotic resistance in *Y. pestis* and to apply this information towards the development of rapid, deployable antibiotic resistance assays. For the purpose of this work, *Y. pestis* isolates with genomic mutations conferring clinically relevant ciprofloxacin resistance were generated by passing an avirulent strain of *Y. pestis* through successive rounds of ciprofloxacin selection. Each round of selection proceeded as follows: inoculate colonies from a parent isolate, plate inoculation onto ciprofloxacin at threefold the minimum inhibitory concentration (MIC) value of the parent, isolate surviving colonies and determine the post-selection MIC value of each new isolate. Preliminary results showed that the ciprofloxacin resistance of *Y. pestis* increased dramatically with each round of selection. After one round of selection, isolates were 20-fold more resistant than wild-type *Y. pestis* (average increase of 27 isolates), and after two rounds of selection, isolates were 60-fold more resistant than wild-type *Y. pestis* (average increase of 26 isolates). Upon completion of a third and final round of ciprofloxacin selection, NimbleGen™ full-genome tiling microarray or Solexa™ full-genome sequencing will be used to identify the genetic differences among increasingly antibiotic resistant isolates, and rapid DNA-based resistance assays will be developed based on the changes identified.

Metabolic Engineering of *Alicyclobacillus acidocaldarius* to make Lactic Acid

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Alicyclobacillus acidocaldarius is a gram-positive bacteria found in thermal features in Yellowstone National Park. It grows at 60 °C and a pH of 4.0. *A. acidocaldarius* has been found to aid in the production of lactic acid, a chemical that can be used to make biodegradable plastic. Currently, the process for making lactic acid is costly and generates waste which comes from the need to perform acid pretreatment on the plant matter that is used as a starting material. After the acid pretreatment, the solution needs to be neutralized and cooled before enzymes that break down sugars into lactic acid can be added. If *A. acidocaldarius* is used, the liquid from the acid pretreatment will not have to be cooled or neutralized as extensively and the bacteria will break down the sugars directly into lactic acid, cutting out intermediate steps while reducing waste and cost. In order for the bacteria to make lactic acid, the cells must produce excess lactate dehydrogenase (LDH), an enzyme that converts pyruvate into lactic acid during carbon metabolism. *A. acidocaldarius* does not make excess LDH under normal conditions, so an LDH gene must be inserted. The purpose of this study is to insert a plasmid containing an antibiotic resistance gene and a controllable LDH gene into the bacteria to aid in the production of lactic acid. This is done by mating *A. acidocaldarius* with *Escherichia coli* cells that contain the plasmid. The two types of bacteria are grown overnight, combined, and then passed through a filter to get the cells in close proximity. To select for cells with the plasmid, the filter is then incubated on agar at 37 °C overnight, and the cells are suspended from the filter into liquid medium, plated on agar with antibiotic added and incubated at 60 °C. This is done in hopes that the *E. coli* cells will transfer the plasmid to *A. acidocaldarius*. Unfortunately, no plasmid transfer was seen. This could be due to unfavorable conditions; mating at pH 5.5 and 37 °C, while optimal for *E. coli*, is not optimal for

A. acidocaldarius, making the cells incapable of receiving DNA. It is also possible that the plasmid is transferred but can't replicate in *A. acidocaldarius*. The goal of expressing LDH in order produce lactic acid will not be met until a system for getting DNA into the cell is developed. In the future, constructing a plasmid that contains native genes from *A. acidocaldarius* may be helpful because it is likely that the plasmid will be more easily accepted by the bacteria.

Elevated Carbon Dioxide Alters Root and Hyphal Decomposition: Implications for Soil Carbon Storage

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Atmospheric carbon dioxide concentrations (CO_2) are 22% greater now than 47 years ago and are expected to continue to increase throughout this century. Elevated CO_2 can increase fine-root (roots less than 1 mm in diameter) production in temperate deciduous forests. Fine roots often form symbiotic relationships with mycorrhizal fungi to maximize nutrient uptake. We predicted that increased fine-root production in the Oak Ridge National Laboratory (ORNL) Free-Air CO_2 -Enrichment (FACE) experiment in eastern Tennessee would lead to an increase in the mycorrhizal hyphae net biomass production, and show that hyphae would decompose at a faster rate than fine roots, leading to differences in the amount of carbon (C) stored in the soil. We tested our hypotheses by quantifying mycorrhizal hyphae net biomass production under ambient and elevated levels of atmospheric CO_2 at ORNL FACE. Hyphal in-growth bags consisting of sand wrapped in 50 μm mesh were inserted into treatment plots in October 2006 and collected in May, September and November 2007, and representative root samples from each plot were collected in June 2007. After hyphal and root production were quantified, potential C mineralization was measured by quantifying the amount of CO_2 respired from incubated roots or hyphae in the laboratory. Contrary to what we predicted, net hyphal production was not greater under elevated CO_2 . More C was available for mineralization in hyphae collected from elevated CO_2 plots than from hyphae collected from ambient CO_2 plots, as well as fine roots from both treatments. Further, the C mineralization rate declined over the course of the incubation more quickly in fine roots grown under ambient levels of CO_2 than those grown under elevated CO_2 , as well as hyphae grown under both treatments. We conclude that under elevated levels of CO_2 , increased fine-root production might lower the reliance of trees on mycorrhizal mutualisms. Further, our findings suggest that while different atmospheric CO_2 treatments alter both hyphal and fine-root C mineralization early on, over time these rates converge. In conclusion, changes in the ratio and decomposition rates of fine roots compared to mycorrhizal hyphae under elevated CO_2 may affect soil C storage, but more studies are needed to measure long-term effects and the ability of forests to mitigate global climate change.

Effects of Cigarette-Smoke Cadmium on the Release of Calcium from Bones in Humans

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Chronic smoking and exposure to second-hand smoke containing cadmium (Cd) have been linked with development of osteoporosis, a metabolic bone disease. Effects of Cd on bone calcium (Ca) release are of great importance and interest to the general public. Calcium is important in maintaining calcium homeostasis, overall bone density and health, and is pertinent in bone growth and strength. Though Cd may be ingested from one's diet or inhaled through cigarette smoke, the gastrointestinal (GI) tract is a much more efficient barrier to Cd than the lungs. Samples of whole blood, blood plasma and urine were collected from volunteer participants once a month for three consecutive months and stored in nitric acid-washed, Cd-free tubes. Samples were analyzed for Cd concentrations by using a low-volume, high-sensitivity assay and an atomic absorption spectrophotometer. Preliminary results show significantly higher whole blood Cd concentrations in female smokers (1.30 ± 0.28 ng Cd/ml, $n=11$; mean $\pm$ SE) and male smokers (1.26 ± 0.32 ng Cd/ml, $n=5$) than female nonsmokers (0.34 ± 0.06 ng Cd/ml, $n=6$). The average Cd ingestion through diet is 2156 ± 810 ng Cd (mean $\pm$ SE) for both smokers and nonsmokers. The four-fold increase in whole blood Cd concentrations of the female smokers demonstrates that the barrier produced by the GI tract is more efficient than the barrier produced by the lungs. Qualitative Ultra Sound (QUS) heel bone scans were taken from participants to determine bone density and relative risk of osteoporosis. Z-scores, which account for age differences, were significantly lower in smokers who smoke 15 or more cigarettes per day than the average female nonsmoker, consistent with the hypothesis that low-level Cd exposure may cause bone loss by a decrease in bone mineral density.

Protein Purification of Various Target Proteins.

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The Midwest Center for Structural Genomics is developing effective methods to determine protein structures in a high-throughput process. The high-throughput process passes through three groups: cloning, purification and crystallography. Proteins required for scientific research are over-expressed in bacterial cells. Protein crystallography is an area of science that takes advantage of the technology of the bacterial cells. Cloning grows the proteins of interest in *Escherichia coli* cells. Purification breaks the cells open through sonification, and the contents are centrifuged on over 16 proteins. The supernatants are then passed over a series of nickel purification columns. The histidine tag is removed by the nickel columns, isolating the protein of interest in the purest form possible. The protein is concentrated and set up in crystallization trials to screen for protein crystals. Some of the crystallization trials include Index, Wizard and Nextel. Each of these trials is set-up in a 96-well Greiner plate. When these are successfully grown, then data collection, data processing and three-dimensional structure solution are attempted.

The Effects of Climate on the Daily Divergence and Habitat Selection of *Bufo woodhousii* Toads

Steven Cudney (DEPAUW UNIVERSITY, GREENCASTLE, IN 46135), Janelle Downs (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352). Amphibian populations are declining globally. As a result, it is important to characterize the habitat selection and daily dispersal of amphibian populations. For this study, five male *Bufo woodhousii* toads in southeastern Washington were radio-tagged in the breeding season and tracked for seven consecutive days and nights. It was predicted that toads would travel further on days that minimized temperature and maximized relative humidity and shade. During the day, the toads dispersed away from their breeding pools and were in habitats that minimized temperature and maximized relative humidity, litter and vegetation height. At night, the toads returned to the same location as the previous night and were in an inundated habitat 89% of the time and were typically concentrated in sections of the breeding pool with more grass. Contrary to initial predictions, the daily distance traveled for each toad was not related to relative humidity ($R^2=0.061$), air temperature ($R^2=0.093$), or soil temperature ($R^2=0.0002$). Overall distance traveled was significantly correlated with toad snout-to-vent length ($R^2=0.64$), mass ($R^2=0.97$) and right calf girth ($R^2=0.91$).

Sample Preparation for High-Throughput Proteomic Studies of the Genus *Populus*

Geoffrey Dann (UNIVERSITY OF WASHINGTON, SEATTLE, WA 98105), Kim K. Hixson (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352). Most *Populus* proteomic work to this date has been done using 2-D gels to excise and analyze specific and desired proteins. Most of these other protocols rely on a protein precipitation step followed with resolubilization using the detergent sodium dodecylsulfate (SDS) followed by electrophoresis separation. However, for high-throughput proteomics it is ideal to keep the sample in a liquid phase all throughout preparation. For the downstream mass spectrometric analysis we cannot use the SDS to resolubilize proteins in the samples since it interferes with analysis. Initial results from a bicinechoninic acid assay (used for protein quantization) and size exclusion chromatography of digested leaf lysates indicated that a large amount of quinones in the sample were obscuring analysis due to covalent modification of the proteins. To inhibit these reactions, three chemicals were analyzed to see which chemical or chemical combination worked best at inhibiting the quinone formation. Leaf samples of *Populus tremuloides* were lysed and resultant protein were digested in the presence of: sodium metabisulfite as an antioxidant, polyvinyl polypyrrolidone to bind polyphenols and Roche brand protease inhibitor to prevent natural protease activity and polyphenoloxidase activity. Results from gel electrophoresis and staining demonstrate that the combination of all three of these materials was most successful in producing protein material as observed from having the highest protein band resolution after gel staining.

Selection and Characterization of c-Myc-Binding DNA Aptamers

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Cancer is a disease that results when cellular processes begin to function outside normal parameters. One of the ways in which a cellular process can be shifted into an abnormal mode is by the deregulation of oncogenes, which are protein-encoding genes that participate in the onset and development of cancer. One such oncogene, called c-Myc, leads to the expression of the c-Myc transcription factor. The c-Myc transcription factor must form a heterodimer with the Max protein in order to bind its target DNA sequence, CACGTG, which is called the

E-box domain. In previous studies, a DNA aptamer was selected using a SELEX (Systemic Evolution of Ligands by EXponential Enrichment) protocol, which identified a segment of single stranded DNA that could bind the c-Myc:Max heterodimer [MNH] with high affinity ($KD=100nM$). However, the affinity for c-Myc is still 100–1000-fold lower than the best reported aptamers. Therefore, its affinity can probably be lowered by molecular optimization procedures. This study is being conducted to characterize the c-Myc aptamer, as a part of the process that will ultimately lead to its optimization. The results of this study will be to develop an aptamer that can be used in future medical treatments, and that can be used to elucidate the mechanisms involved in the cancer pathways resulting from the unregulated functioning of c-Myc.

Mechanical Changes Occurring During Poplar Cell Wall Growth

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Finding a cost-effective, sustainable alternative to fossil fuels is a major concern due to both political and environmental pressures. The production of ethanol from plant materials offers an alternative; however, existing technologies using corn are neither cost-effective nor environmentally sustainable. Cellulosic ethanol offers an alternative to corn ethanol. Cellulose is the most abundant polymer found in nature but cellulosic ethanol is still expensive to produce due to the difficulty of extracting cellulose from plant cell walls. At this time, there are many questions about plant cell wall structure that are still unanswered. One area of research concerns the development of the cell wall. To further understand some of the changes occurring during cell wall growth, poplar protoplasts were obtained. One sample was kept at 4 °C, the other kept at room temperature for 24 hours to allow the initial formation of a cell wall. These samples were then imaged using both atomic force microscopy and scanning near-field ultrasound holography. To assess changes in relative stiffness, force curve measurements were taken. It was found that cells that had begun cell wall growth were stiffer than those that had not yet begun cell wall growth. Furthermore, it was observed that there were distinct visual changes that corresponded with changes in mechanical properties. Although there are not yet enough samples to make this finding statistically significant, these data suggest that there are mechanical changes occurring during cell wall growth. In the future, more data will need to be taken and correlated with molecular changes occurring during cell wall growth.

Characterization of Poplar and Switchgrass by Atomic Force Microscopy

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Finding a cost-effective, sustainable alternative to fossil fuels is a major concern. Current methods of ethanol production are energy-negative — they actually increase our fossil fuel consumption. Cellulose is the most abundant polymer found in nature but cellulosic ethanol is still expensive to produce due to the difficulty of extracting cellulose from plant cell walls. Cellulose is located in the cell walls of plants within a matrix of lignin and hemicelluloses. This matrix is not yet well understood and is what makes the extraction of cellulose so difficult. More basic information about the molecular composition of cell walls is needed to develop cost-effective technologies for ethanol production. To help address the deficit in basic information about cell wall composition, we focused on analyzing cell wall materials using atomic force microscopy (AFM), which has nanometer-scale resolution. We prepared multiple samples of poplar wood and switchgrass. The samples were prepared for imaging by mounting shavings of switchgrass and poplar on a slide using epoxy. Images were then taken of these samples. The images obtained are remarkably similar to an earlier experiment done at the University of Miami in which lignin monomers were allowed to self-assemble on a cellulose substrate. In light of this literature, we propose that the images we have garnered are in close accordance with the lignocellulosic structure. In the future, more high resolution images need to be obtained. In addition to AFM images, we are working on experiments that include obtaining data by Fourier transform infrared spectroscopy and Raman spectroscopy. When the data from all of these experiments are combined, we should be able to gain a broader understanding of the molecular architecture of cell walls which may one day shed light on the challenge of efficient cellulosic ethanol production.

Rapid Methods of Detecting Molecular Changes Associated with Antibiotic Resistance in *Yersinia pestis*

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The spread of antibiotic resistance in pathogens poses a threat to global health and security, especially as current drugs or dosages

become ineffective. *Yersinia pestis*, causative agent of the plague in Medieval Europe, is now treatable by several antibiotics but would still have epidemic potential if it acquired resistance to these antibiotics. This project seeks to identify how molecular changes and DNA sequences are affected by antibiotic concentration and apply this in an assay for the detection of antibiotic resistance. In order to acquire clinically-relevant antibiotic resistant isolates, an avirulent strain of *Y. pestis* was taken through three rounds of selection. Each round selected for a threefold increase in antibiotic resistance compared to the minimum inhibitory concentration (MIC) of the parent isolate. Thus far, thirty isolates have been taken through two rounds of selection, showing an average of a twentyfold increase in MIC values in the first round. Extrapolating into the third round, it is likely that mutants will have a MIC values higher than the recommended clinical dose of ciprofloxacin for plague treatment, which demonstrates the ease and danger of amplifying antibiotic resistance. When there is a sufficient number of antibiotic resistant isolates, NimbleGen™ microarray or Solexa™ full-genome sequencing will be performed to locate changes in DNA sequences between resistant isolates and the original strain. Finally, Taqman (DNA-based, polymerase chain reaction) assays will target the specific mutations and will be validated against resistant and sensitive strains.

Effects of In Vivo Exposure to Chlorpyrifos and In Vitro Exposure to Chlorpyrifos Oxon on Cholinesterase Activity in Lungs of the Rat *Rachael Fox (TRINITY WESTERN UNIVERSITY, LANGLEY, BC V2Y 1Y1), Andrea Busby (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352).*

Chlorpyrifos (CPF) is a pesticide that is generally applied using an aerosol spray which can be inhaled, exposing the lungs of agricultural workers to CPF. Upon entry to the body, CPF can be metabolized to produce the toxic chemical chlorpyrifos oxon (CPO). CPO binds to cholinesterase (ChE), inhibiting it from regulating acetylcholine (ACh) levels in the body. Though inhalation is one of the primary routes of exposure, little is known about the effects of CPF on lung ChE activity. The focus of this study is to determine effects on lung ChE activity from exposure to CPF and CPO. In this study untreated lungs were analyzed using the Ellman assay to determine their total ChE activity. Control lung samples were analyzed using the Ellman assay and two different substrates (acetylthiocholine chloride [ATC] and butyrylthiocholine iodide [BTI]) to determine the relative activities of acetylcholinesterase and butyrylcholinesterase, two types of ChE. Lung tissue was incubated with varying concentrations (1–10 000 nM) of CPO to find the concentration of CPO that causes 50% inhibition of ChE activity (IC_{50}). Lungs from rats that had been treated in vivo subcutaneously with 10 mg/kg CPF and lungs from rats that had been treated in vivo with an oral dose of 4.91 mg/kg were analyzed using the Ellman assay to determine the percent inhibition of their ChE activity. Average total activity in lungs at a dilution of 1/300 was found to be 14.5% of the total activity in brain at a dilution of 1/1750. Average ChE activity in lung when BTI was used as a substrate was 43.8% compared to the activity observed when using ATC as a substrate. IC_{50} values for lung tissue were determined to be at 76.5 and 52.7 nM concentrations of CPO using ATC and BTI as Ellman assay substrates, respectively. ChE activity in lungs of animals treated subcutaneously with CPF had 72.8% activity compared to control lungs. Lungs of animals treated orally with CPF had 52.5% activity when compared to control lungs. This data shows that in vivo CPF exposure and in vitro CPO exposure affect the activity of ChE in lungs, and demonstrates the need for future studies investigating the effects of CPF and CPO on lungs.

Purification and Characterization of the Gln115A Mutant of the Human Adenovirus Proteinase

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The adenovirus proteinase (AVP) is an essential enzyme involved in the maturation of the virus. An active proteinase is required for the virus to become infectious. Previous study has revealed the crystal structure of wild-type AVP. The crystal structure placed a glutamine at the 115th residue (Gln115) near the oxyanion hole. The oxyanion hole is responsible for orientation of the peptide bond in the correct position for catalysis to proceed and also helps in stabilizing the transition state during the bond cleavage reaction. Therefore, a mutation at the 115th residue from a glutamine to an alanine (Q115A) should have greatly impaired AVP activity. This study investigated the effect of the Q115A mutation. Mutagenesis was done previously by Quick-Change and the mutant gene was put into the pET13a expression vector and electroporated into *Escherichia coli* cells. The mutant AVP was verified to be present in soluble form by SDS-PAGE and was purified first through a cation exchange column, and then through a hydrophobic-interaction column. The mutant's mass was verified by MALDI mass

spectrometer to be consistent with calculations. Activity assays were performed with an artificially synthesized Rhodamine fluorescent peptide substrate. The mutant had no apparent activity by itself, but showed minor activity in the presence of pVlc, an important cofactor for AVP. The catalytic rate was further increased with the addition of DNA, another cofactor. The mutant showed at least 200-fold less activity than wild-type AVT in the presence of both cofactors. Future study is to crystallize the mutant protein and its complex with substrate to determine if the reduction in activity is due to folding error. Since the mutation had greatly reduced enzyme activity, the Gln115 site is a possible target for anti-viral drugs.

Development of Bioforensic Methods for *Brucella abortus*

Michalena Grosshans (OHIO NORTHERN UNIVERSITY, ADA, OH 45810), Francisco F. Roberto (IDAHO NATIONAL LABORATORY, IDAHO FALLS, ID 83415). A simple and reliable method for detecting the zoonotic bacterial pathogen *Brucella* is essential for the diagnosis and containment of the infectious disease brucellosis. Various *Brucella* species, which infect animals, may be transmitted to humans. In the United States, *Brucella* is primarily found in animals, especially in the Greater Yellowstone Area where one species, *Brucella abortus*, is endemic to elk and bison populations and can spread to cattle. *B. abortus* causes cows to abort their fetuses and renders their meat inedible. In the event of an outbreak, a state loses its 'brucellosis-free' status and ranchers must slaughter the infected cattle. *Brucella* also poses a threat as a biological warfare agent and is considered a possible terrorist weapon. This work was aimed at developing a species-specific assay for *B. abortus*, which in time could help create better vaccines and treatments and would be useful in the event of a human outbreak. Initially, fast real-time polymerase chain reaction (PCR) was performed. Two primer/probe sets (Bab1 and Bab2) were designed and tested for specificity against a panel of fifteen DNA strains — both *abortus* and non-*abortus*. Bab2 was rejected for non-specificity. Further trials of Bab1 used broader DNA panels. Primer and probe concentration optimization tests analyzed a matrix of primer concentrations at 50, 300 and 900 nM and probe concentrations ranging from 50 to 250 nM. Sensitivity testing used serial dilutions of DNA from 500 pg to 0.5 fg, and intermediate dilutions below 50 fg. In an effort to attain greater sensitivity, the assay was tested on a non-fast block instrument using the optimized protocol. Results showed that the non-fast block method provided more reliable results. Consistent detection has been achieved at as low as 15 fg, equivalent to approximately three genomic copies, on both the fast block and non-fast block machines. Optimization tests allowed the use of concentrations of the primers and probe below the standard protocol, making the assay more cost effective. Use of the non-fast block instrument means the assay is more time-consuming than fast PCR; however, it provides more consistent results and still offers a significant time advantage over end-point PCR. Also, real-time PCR can quantify the amount of target present. Future work is needed to validate the assay, however, results are promising that it could be useful to diagnose the presence and quantify the amount of *B. abortus* in unknown samples.

Microbial Diversity in an Extremophilic Biofilm

Alicia Gunterus (DIABLO VALLEY COLLEGE, PLEASANT HILL, CA 94523), Tamas Torok (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). Exploring biological diversity leads to the detection of new microorganisms with novel traits beneficial to environmental and industrial applications. Hyperthermophilic organisms are of great interest because they have unique characteristics enabling them to survive at high temperatures with minimum nutrients, and hence are suitable for novel biotechnology applications. The purpose of this study was to characterize microorganisms that formed a biofilm at an active fumarole site. Analysis was based on small subunit ribosomal RNA-gene sequences using DNA microarray technology and SEM and TEM electron microscopic imaging. A total of two archaeal and 36 bacterial phyla were detected in the biofilm sample, representing two archaeal and 115 bacterial families. The most abundant phylum was *Proteobacteria*. Photosynthesizing chlorophyll *a*-containing cyanobacteria caused the deep green color of the biofilm top layer, while anoxygenic photosynthesizing proteobacteria gave the middle layers colors ranging from purple, red, brown to orange. Less biological activity was found at deeper layers. SEM and TEM images revealed a diverse microbial community and indicated that all layers of the biofilm were dominated by tubular structures of cyanobacteria. Presence of lamellar thylakoid membrane structures was frequently observed. Cells were intensely embedded in extracellular polymers. Images were rich with vesicle formations and fibrous extracellular structures.

Ionic Liquid Pretreatment of Lignocellulosic Biomasses for Enhanced Saccharification

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With depleting supplies of petroleum-based fuel, there is increasing demand for renewable transportation fuel. Cellulosic biomass has great potential to meet the demand, but biomass must be pretreated to unlock the trapped energy. Pretreatment is essential since plant cell wall cellulose, which can be converted to sugar by saccharification to produce biofuel, is highly crystalline and protected by its complex network of lignin and hemicellulose. Current pretreatment methods are inefficient in breaking down the cell wall or producing inhibitory glucose and xylose degradation products which inhibit the enzymatic hydrolysis of biomass fermentation into sugar. Ionic liquids are green solvents and show great potential in solubilizing cellulose. However, it is not clear how lignin solubilizes cellulose, hemicellulose and lignin. The overall goal of this study is to examine how lignocellulosic biomass breaks down in ionic liquids via hydrolysate analysis in order to increase yield and mitigate the formation of inhibitory compounds, thereby decreasing the cost of operation associated with cellulosic ethanol production.

Poly(N-isopropylacrylamide-co-Acrylic Acid) Scaffolds Prepared with Nerve Growth Factor as a Transfer System for the Treatment of Parkinson's Disease

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Parkinson's disease (PD) is a progressive neurodegenerative disorder of dopaminergic neurons in the nigrostriatal pathway that affects millions of people worldwide. Cellular replacement therapy as a mode of neuroregeneration for PD has shown promise, but viability and survival rate of grafted tissue is a primary issue of concern. Poly(N-isopropylacrylamide-co-Acrylic Acid) (PNIPAm-co-AAc), a biocompatible three-dimensional scaffold with a phase transition near in vivo temperature, may combat these issues by mimicking the neuronal microenvironment. The focus of this study was to enhance survivability of grafted cells and consequently improve proliferation and dopaminergic differentiation by culturing cells in PNIPAm-co-AAc prepared with nerve growth factor (NGF). Rat glioma cells (3RT1) transfected with green fluorescent protein (GFP) and rat pheochromocytoma cells (PC12) were cultured and incubated at 37 °C in Dulbecco's Modified Eagle's Medium and Ham's F12K medium, respectively. Both cell lines were then seeded into the polymer scaffold, which was formulated with phosphate buffered saline (PBS). The cell/polymer mix was then injected into warm media. For PC12 seeding, NGF was added to the matrix and cellular response to NGF-mediated outgrowth was scored by observing both the rate of morphological differentiation and the extent of neurite outgrowth. Due to the opaque nature of PNIPAm-co-AAc, GFP was used to visualize neurospheres within the scaffold by exciting GFP at 488 nm using a green fluorescent light. We observed that PNIPAm-co-AAc scaffolds provided a worthy environment for the adhesion and growth of cells. The scaffold prepared with NGF permitted the differentiation of PC12 into a neuronal-like morphology, which is presumed to have increased excitability. This approach allows for the possibility of transplanting cells through a surgical catheter. Once in vivo, the hydrogel can become a three-dimensional network providing structure and assisting in proliferation and differentiation into dopamine producing neurons.

Study of Cell Wall Decomposition of Yellow Poplar by Microbial Activity

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The tough matrix of cellulose, hemicellulose and lignin composing a plant's cell wall poses a major obstacle to the fermentative production of alternative fuels and chemicals from biomass. This wall has to be broken down in the pretreatment of the biomass. Because plants' cell walls contain a major portion of the biological carbon present on the earth at any one time, microorganisms have evolved a diverse array of enzyme catalysts that are effective in dismantling and recycling this complex material. It was proposed to perform a comprehensive study of the natural degradation of biomass by microbes. This study would be conducted using a composter and would be the first of its kind conducted at the National Renewable Energy Laboratory (NREL). The insights gained about the enzymes used during the breakdown could lead to future research taking advantage of this information for the pretreatment process of fermentative ethanol. During the course of this research a composting process was developed and carried out, microscopy was utilized to analyze the samples collected during

the course of the composting, and the gene expression of enzymes involved in the biomass degradation was studied in great detail through the use of real-time polymerase chain reaction (PCR). The microscopy showed compelling evidence of the breakdown of the hemicellulose and lignin in the cell wall, thereby exposing the cellulose. The PCR experiments produced a library of primers that will be used to continue screening of compost samples. A total of 20 successful and specific primer sets were designed, with 12, 6 and 4 primer sets targeting genes encoding cellulose-, hemicellulose- and lignin-degrading enzymes, respectively. Future research will concentrate on profiling of the selected genes encoding cellulolytic enzymes over the time-course of composting.

Imaging Diatoms with Atomic Force Microscopy

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Diatoms are unicellular, eukaryotic microalgae that use silica and organic materials to make intricate skeletons, referred to as frustules, with nanoscale features. There is much to learn about how diatoms fabricate these structures. We are using high-resolution atomic force microscopy (AFM) to image 16 different species of diatoms, in various stages of their development, to better understand how these organisms fabricate their cell walls. The diatoms in this study were acid cleaned to remove organic substances, then suspended in water. We prepared samples for AFM analysis by spotting 10 μ L of the suspensions on gelatin-coated mica and allowing the liquid to air dry. Imaging was done in contact mode using a PicoPlus AFM (Molecular Imaging, Tempe AZ), with a silicon nitride cantilever with a spring constant of 0.1 N/m. The images produced in this study revealed microscale features and nanoscale textures of the frustules, including girdle bands, valves and setae of many different species of diatoms. The images highlight both overall structural themes and diverse species-specific structures. Images of valves and girdle bands showed that these structures often have proximal and distal surfaces with different textures, indicating a three-dimensionality in their formation. The diatom surface topology that was revealed in this study provides insight into the underlying organic materials involved in frustule formation. Additional work will image diatoms with chemically functionalized AFM tips; this is expected to chemically map frustule surfaces, which should increase our understanding of cell wall fabrication. Understanding how diatom structures are produced could provide fundamental knowledge leading to more efficient nanofabrication methods, with applications in many fields including catalysis, photonics and robotics.

Development of Enzyme Assay Method for High-Throughput Detection of Endoglucanase Activity

Shih-Yao Hsu (UNIVERSITY OF CALIFORNIA—LOS ANGELES, CA 91001), Rajat Sapra (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). Manufacturing cellulosic ethanol efficiently and cost-effectively was the ultimate goal of researchers at the Joint BioEnergy Institute (JBEI). The JBEI Enzyme Engineering Group in the Deconstruction Division at this facility aims to engineer cellulase that effectively breaks down cellulose into glucose, which can be converted into cellulosic ethanol. This protein engineering work on cellulase enzymes strives to produce mutant enzymes that have better catalytic activity than the wild-type enzymes. Although there are various enzyme assay methods available to detect cellulase activity, there is a need to engineer robust enzyme assays that are both sensitive and quantitative for measuring cellulase activities of thousands of mutant enzymes in high-throughput format. In this project, commercially available cellulases were used to examine established cellulase assays based on glucose hexokinase (HK), Congo red and azo-carboxycellulose (Azo-CMC). Additionally, Remazol Brilliant Blue R (RBBR), the dye used in Azo-CMC assay, was tested for absorbance vs. concentration ratio and optimum scanning wavelength. HK assay results showed a consistent linear range for the glucose concentration of 0 to 7.5 mM. The Congo Red assay plot demonstrated no significant difference in cellulase activity on agar plates of different pHs. Azo-CMC assay data indicated linear section in cellulase concentration below 0.5 mg/ml or 0.00225 enzyme activity unit. Lastly, results from RBBR suggest that there is a definite linear trend from 1 μ m to 750 μ m RBBR with extinction coefficient value of 4346.3 M⁻¹cm⁻¹ and that wavelengths of 590 nm were optimum.

20S Half Proteasome Purification and Crystallization

Mengyin (Cassie) Hu (UNIVERSITY OF CALIFORNIA—BERKELEY, BERKELEY, CA 94720), Huilin Li (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Mycobacterium tuberculosis (Mtb) is the bacteria that causes TB. The difficulty in treating TB infection is largely due to Mtb's unusual ability to survive inside the human macrophage. The 20S proteasome is a highly conserved protein assembly that plays many essential roles in a cell, such as degradation of other proteins and control of cell cycle. Mtb has

a hard time surviving in the macrophage without its 20S proteasome. The proteasome structure contains two type of proteins — the alpha- and beta-subunits, which form four rings in a 7b7b7a7 order, with seven subunits in each ring. The 20S proteasome is assembled from two half proteasomes during which the pro-peptides of beta subunits are autocleaved to expose the active amino terminal threonines. Although the crystal structure of the full proteasome is known, the structure of the half 20S proteasome, the location of its pro-peptide, is unknown. Our research plan was to crystallize the half 20S and to use the X-ray beam at the National Synchrotron Light Source in Brookhaven National Laboratory to probe the crystals of the half 20S in order to get the diffraction data needed for solving its atomic structure. After multiple trials, we found that the bacteria expressed our target proteins in the form of half 20S proteasome 18 hours after addition of an expression inducer in the culture media. By using the Ni-NTA affinity and the gel filtration chromatography, we were able to purify the half 20S in the 4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid (HEPES) buffer. Importantly, we were able to obtain crystals of the half 20S proteasome. Although crystallization condition was not fine-tuned at this point to improve the quality of the crystals, results have nevertheless laid a solid foundation for further experimentation.

Effects of Ubiquitin-Specific Proteases (USPs) on *Aspergillus niger* Morphology and Citric Acid Production

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Citric acid is a weak organic acid that is responsible for the tart taste characteristic of many fruits. A popular food additive and an important intermediate in the citric acid cycle, citric acid is one of the most widely produced organic acids by fermentation with the filamentous fungus *Aspergillus niger*. High production efficiency is often associated with growth as small pellets. While the exact regulatory mechanisms that control fungal morphology are still inadequately defined, previous studies suggest that the ubiquitin system is one of the molecular pathways that are responsive to the effects of Mn²⁺ concentration on *A. niger* morphology. The deubiquitylating enzymes are a critical component in the ubiquitin system and mediate the removal and recycling of the ubiquitin unit inside the cells. The ubiquitin-specific proteases (USPs) represent the largest subclass of deubiquitylating enzymes and may play a role in regulating morphology and citric acid production. In this study, three putative USPs (USP3, USP5 and USP44) were examined by gene deletion analysis, which involves building constructs that consist of the upstream regions of the target genes, the hygromycin marker gene and the downstream regions via double joint PCR. Insertion of the transgene constructs into *A. niger* cells was accomplished via protoplast transformation. After several days of growth on plates, the hygromycin resistant mutants were selected and further grown in culture tubes for spore production. The spores were collected and cultured for biomass from which genomic DNA was extracted. The genomic DNA was used for PCR screening to confirm the successful deletion of the USP3, USP5 and USP44 genes in the hygromycin resistant mutants. Upon final confirmation of gene deletion via Southern blot, the fungal mutants will undergo phenotypic analyses, where they will be observed for any changes in their morphology and organic acid production rates. The results from these studies will aid in establishing the roles of USPs in the growth and development of filamentous fungi.

Analysis of Biomimetic Lanthanide and Actinide Decorporation Agents in Human Renal Cortical Epithelial Cells

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Two synthetic ligands that can chelate radioisotopic contamination in the human body have recently been developed by Dr. Kenneth Raymond, Senior Faculty Scientist at LBNL and Professor of Chemistry at the University of California—Berkeley. These agents could be extremely useful to treat victims of terrorist events exposed to radioisotopes in a "dirty bomb." The two new ligands that have shown significant efficacy in chelating actinides are 5LiO (5LiO-Me-3,2-hydroxypyridinone) and 3,4,3-Li (3,4,3-Li-1,2-hydroxypyridinone). These ligands are under study for human use to replace the currently used decontamination agent Ca-diethylenetriaminepentaacetate (DTPA). In vitro cellular toxicity studies are needed to determine the impact of 5LiO and 3,4,3-Li in the primary filtration organs of the human body. This report describes a series of experiments designed to determine the inherent toxicities of these drugs. The 3-[4,5-Dimethylthiazol-2-yl]-2,5-diphenyltetrazolium bromide(MTT), Trypan Blue and Alcian Blue Viability assays were utilized to assess cell viability after six-hour drug challenges and 24-hour recovery periods in early passage human renal cortical epithelial

cells. Further experimentation in other cell lines and error analysis of data from three replicate experiments are currently in progress. The two ligands under study in this investigation are much more effective in chelating actinides and at much lower drug doses than the currently accepted Ca-DTPA.

Purification and Crystallization Strategies for Novel Proteins Cloned in Vector pMCSG19

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The Midwest Center for Structural Genomics (MCSG) at Argonne National Laboratory produces milligram amounts of reproducible and homogenous protein samples. The proteins' three-dimensional structures are then determined through the use of synchrotron X-ray crystallography at the Advanced Photon Source. *Escherichia coli* BL21 (DE3) is cloned using vector pMCSG19. By conducting proteomic research on cloned proteins with minimal sequence similarities and unidentified properties, one hopes to identify and gain a better understanding of protein function and interactions through computational predictions and subsequent enzymatic assays. This, in turn, can lead to the utilization of said proteins in commercial applications in the environmental, medical and pharmaceutical industries. Protocols for the high-throughput (HTP) protein purification pipeline include the use of a histidine tag, subsequent cleaving using the Tobacco etch virus protease (TEV), and immobilized metal affinity chromatography (IMAC). Protein purity is assessed using polyacrylamide gel electrophoresis in the presence of sodium dodecyl sulfate (SDS-PAGE). The use of automated robotics that have minimal human interaction, including the AKTA Xpress workstation, which carries out multidimensional chromatography, are heavily implemented. Additionally, solubility tests will be conducted on small-scale and large-scale protein samples to determine if the protein is viable for experimentation prior to the purification process. The MCSG high-throughput protein purification pipeline protocol will be discussed in this paper. Optimization of crystallization methods will also be explored and explained on proteins that fail to crystallize or produce a defined structure.

Advanced Protein Purification and Crystallization Identification Using High Performance Chromatography

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The purpose of the research performed by protein purifiers in the Biosciences Division at the Structural Biology Center (SBC) is to collect a sample of protein completely free of contaminants so that a correct crystallized form of that protein can be obtained. By determining a protein's three dimensional structure, researchers are able to understand its functionality within its natural state and the affects/consequences it has based on its tertiary folding. The SBC has established three different teams working cohesively, whose sole purpose is to develop proteins, purify protein and to determine the validity of that protein's structure. Using synchrotron X-ray crystallography, the three dimensional structure of protein can be determined. Based on the SBC procedure and protocol, all target proteins must fall within a pre-determined range of solubility and expression to ensure the best crystal formation. Since only the purest proteins produce the strongest crystals, the SBC requires the use of high performance chromatography workstations AKTA Xpress and IMAC 2 to ensure as little contamination as possible. This procedure should ensure that once the purified target proteins are exposed to certain conditions it should solidify into a crystallized structure, if not, additional protocols will be implemented to tease forward solidified structures. Once a crystal is formed and identified it is passed on to the crystallographers for structure analysis, the third stage of the SBC protocols.

Engineering Novel Allosteric TMR-Responsive RNA Aptazymes

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Aptamers are RNA sequences that bind to target molecules and consequently regulate gene expression in a ligand-dependent fashion. They are frequently employed in nature to couple fluctuations in the concentration of a metabolite with changes in gene expression. Upon binding a small molecule, aptamers sequester the ribosome binding site [RBS] of a cis mRNA and repress translation. Synthetic aptamers eliminate the need to rely upon pre-existing biological molecules as the source of binding structure. Generation of synthetic aptamers occurs through in vitro selection, iterative rounds of enrichment and amplification which eventually select for an RNA molecule with high binding affinity (~100 μ M) and specificity. Through a combination of

directed evolution and rational design we generated functional, ligand-binding RNA structures that may potentially control the cis-expression of mRNA transcripts in response to tetramethylrhodamine (TMR), a small fluorescent dye that is cell permeable. Iterative rounds of selections and binding assays in in vivo like conditions have generated several isolates of TMR-binding aptamers. When incorporated into constructs with self-cleaving hammerhead ribozymes, such molecules will provide general tools for simultaneously varying the expression levels of toxic intermediates in engineered pathways.

Determination of Temperature Criteria for Snake River Fall Chinook Salmon

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Shoreline pool entrapments are formed in the Hells Canyon Reach of the Snake River when the water flow decreases. This can occur naturally during flood control or during low power demand periods. Fall Chinook salmon spawn in this reach and juveniles which feed and rear can become trapped in these pools during high flow events and are unable to return to the main river channel. During the rearing period fish normally inhabit water temperatures ranging from 10 °C to 14 °C, while pool temperatures during the day can exceed 25 °C. Currently NOAA has the limits set at three days for 16 °C and four hours at 18 °C. The purpose of this study is to determine what the maximum sustained temperature juvenile fall Chinook salmon can tolerate and what the maximum short term temperature is they can tolerate. This was accomplished through the use of 80 six-gallon pails that were used to hold fish at a constant (control) temp and others that increase water temperature during the day to simulate heating of the pools. For the tolerance tests fish were held a minimum of two weeks at 10, 12 and 14 °C to simulate river conditions and then heated 1.5 °C every hour to a maximum at which all fish died in order to simulate pool entrapment. The maximum temperature at which all fish died was 27.5 °C. Additional tests were done to determine the effects of long term exposure to 25 °C. Fish behaviors such as the loss of equilibrium and time of death were determined by using video cameras and a DVR. The project sponsor, Idaho Power Company (IPC), is interested in the impacts of rearing fish below Hells Canyon Dam and if the current regulations are more restrictive than they need, thus allowing them to reduce the amount of non-power generating water past the dam. By gathering data that demonstrates the optimal growth conditions and the levels of mortality caused by temperature fluctuation, a determination can be made about changing the flow requirements during the fall Chinook salmon rearing period. It is possible that the findings of this study may alter the regulation of outflows which correspond to the duration of time that the pools would be isolated from the main river flow and may well spawn other studies to determine the parameters that are acceptable for other species. These new guidelines could alter the level of mitigation necessary by the power companies as more accurate assessments are compiled about juvenile salmonid temperature induced mortality.

Reduction of Uranium (VI) to Uranium (IV) by Microbes at Multiple Depths with the Addition of Electron Donors

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Contamination of environments is detrimental to all living organisms. Unfortunately, there are many contaminated areas, some of which contain uranium. Uranium is radioactive and toxic, which can cause numerous health problems if consumed, for example, through drinking water from a contaminated well. Currently, research is being conducted to reduce U (VI), which is soluble, to U (IV), which is insoluble. My project looked at the impact upon uranium reduction rates by the addition of electron donors for soil samples from different depths. Microcosms were created with soil from five different depths and groundwater from the Natural and Accelerated Bioremediation Research Field Research Center at Y-12. Electron donors, ethanol, methanol and ethanol+pyruvate, were added to some of the microcosms. Samples were taken throughout the experiment to look at nitrate concentration, U (VI) concentration and the microbial community. Ion chromatography measured the nitrate concentrations, which is important because if nitrate is present in the sample then uranium reduction cannot occur. A kinetic phosphorescence analyzer was used to measure the U (VI) concentration. The microbial communities will be determined through functional gene arrays and 16S sequencing. The microcosms with pyruvate reduce U (VI) at a higher rate for most depths. This higher rate of uranium reduction should occur because it is believed that the pyruvate moves U (VI) from within the soil into the water, which provides the microbes easier access to the uranium and thus facilitates their reduction of the uranium. However, the microcosms containing ethanol reduced uranium in this experiment methanol were

not found to promote reduction of U (VI). The microbial community is ongoing and will indicate what microbes are present in the soils and which are likely reducing the uranium. Ultimately, this research will be used to clean up the many uranium contaminated areas throughout the United States and elsewhere

Comparing the Disposition of Perfluorooctanoic Acid Between Gender of Fathead Minnows after Oral Dosing

Jonathan Lee (BRIGHAM YOUNG UNIVERSITY—IDAHO, REXBURG, ID 83460), Irvin Schultz (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352). Perfluorooctanoic acid (PFOA) is molecule composed of a carboxyl group with a 7 carbon chain where there is fluorine bonded to every carbon within the chain. PFOA persists in the environment and can bioaccumulate in aquatic organisms. This bioaccumulation has caused scientists to study the toxic effects of PFOA on organisms. My study characterized the uptake, distribution and elimination of PFOA in fathead minnows (*Pimephales promelas*) after controlled oral dosing. The fish were separated into four groups: female control, male control, females exposed to trenbolone (male hormone) and males exposed to ethynylestradiol (EE2, female hormone). The experiment was performed by orally dosing the fish with *Artemia* that had previously bioaccumulated PFOA to a known level. After various time periods after dosing, the fish were euthanized and their plasma and gonads removed and analyzed along with the carcass for PFOA. My study found that there was a clear gender difference in elimination of PFOA. I found that females removed PFOA faster than males. It was further identified that females pretreated with trenbolone removed PFOA slower than females not exposed to trenbolone and males pretreated with EE2 removed PFOA faster than males not exposed to EE2. These findings suggest that androgens play a role in modulating the bioaccumulation of PFOA in fathead minnows.

Systems Genetics: Elucidating Networks that Underlie Heritable Variation in Adipose Function and Susceptibility to Obesity

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Obesity and its co-morbidities are rampant in Western society. Excess adipose tissue not only physically stresses the organism but also disrupts homeostasis through release of adipokines, bioactive molecules produced in adipose tissue. The long-term goal is to determine the mechanisms by which heritable differences in adipose function impact risk for obesity and its consequences. Systems genetics was employed by anchoring phenotypic variation to naturally occurring genetic polymorphisms in two mouse genetic reference populations (GRPs). These GRPs were recombinant inbred BXD (C57BL/6J X DBA/2J) strains and a panel of eight genetically diverse strains that serve as progenitors for the collaborative cross (CC), an emerging GRP. Body and fat pad weights, plasma hormone profiles and adipose expression of adipokine genes were measured in males of twenty-four BXD strains and in both sexes of the eight CC parental strains. Current progress demonstrates that adiposity is highly correlated with expression of some adipokine genes (e.g., leptin, $r^2 = 0.626$; $p = 5.4E-6$) but not others (e.g., visfatin, $r^2 = 0.012$, $p = 0.937$), a subset of tightly intercorrelated adipokines are regulated independent of adiposity; and sexually dimorphic relationships exist among adipokines and adipose weight. Ongoing assay of adiposity in emerging generations of CC mice confirms that this new GRP will provide physiological diversity reflective of its genetic diversity and on par with that in a human population, highlighting its power to dissect the molecular components of complex traits. Collectively the results suggest that factors in addition to adipose mass need to be considered when predicting genetic risk for conditions co-morbid with obesity.

Gas and Water Flux Through a Carbon Nanotube-Polymer Membrane

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In past studies, carbon nanotubes (CNTs) have exhibited gas and water flux rates significantly higher than Hagen-Poiseuille predicted rates. The smooth, hydrophobic surfaces of the walls provide stranded, frictionless water flow while the small inner diameters of the CNTs (2–10 nm) allow gas to flow in the Knudsen regime with no viscosity. This study aimed to fabricate a CNT-polymer membrane and test it to determine both the net flux and the permeance of gas and water through the membrane. The membrane was fabricated via a polymer-based process. First, CNTs were grown on a silicon support followed by injection of a monomer into the CNT matrix. The monomer infiltrated the gaps between the CNTs and was allowed to polymerize. The membrane was then removed from its silicon support and attached to an aluminum support with epoxy. The final step was opening the CNTs to allow flow through the membrane; this was accomplished with ion

milling, reactive ion etching and water plasma etching. For testing, the membrane was placed in a pressure cell and flow was obtained via pressure-driven permeation. Nitrogen gas flux was tested over a range of pressures up to 8 psi, while water testing occurred at 5 psi. In gas flow testing, the membrane exhibited a linear relationship between volumetric flux and pressure and a permeance that remained nearly constant with increasing pressure. This result indicated pressure dependence consistent with Knudsen permeation, not viscous flow, meaning the gas flow through the membrane was through the CNTs and not through large defects or pinholes in the membrane. The water flux through the membrane was small (less than 0.3 $\mu\text{L/hr}$), and later testing of the pressure cell revealed that approximately half of the observed flow was due to pressure cell leakage, not permeation through the membrane. However, even after correcting for the leak, the water flux through the membrane was still several orders of magnitude higher than Hagen-Poiseuille predictions. Higher net water flux through the membrane could be obtained by increasing the membrane's surface area or decreasing the membrane's thickness. With further developments in membrane manufacturing, the membrane shows great promise for use in future filtration and desalination applications.

In Vitro Metabolism of Chlorpyrifos in Lung and Liver Microsomes

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Chlorpyrifos [O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate, CPF] is a widely used agricultural pesticide that has been extensively studied due to health risks associated with CPF exposure. Metabolism of CPF to its neurotoxic form, chlorpyrifos-oxon (CPF-oxon), results in irreversible inhibition of cholinesterase (ChE) which causes effects such as salivation, diarrhea and tremors. An alternative detoxification pathway produces 3,5,6-trichloro-2-pyridinol (TCP), a relatively harmless metabolite that is readily excreted in urine. Both of these metabolic pathways are mediated by Cytochromes P450 (CYP450). The majority of CPF is metabolized in the liver, but other organs containing CYP450 enzymes may metabolize CPF as well. Investigation of CPF metabolism in the lungs is of particular importance as pesticide workers regularly receive direct exposure to aerosolized CPF. The metabolism of CPF to TCP in lung and liver microsomes was compared to provide a preliminary understanding of the magnitude of CPF metabolism in the lung. Lung and liver microsomes were incubated with CPF concentrations of 50, 150 and 500 μM and 25, 50, 150, 250 and 500 μM , respectively, and the amount of TCP generated was analyzed using gas chromatography/mass spectrometry (GC/MS). This data was used to determine the Michaelis-Menten kinetics of chlorpyrifos metabolism in the lung and liver. The maximum velocity (V_{max}) of lung metabolism was 44% of the liver metabolism. The Michaelis-Menten constant (K_m) of the lung and liver were 5.9 and 21.0 $\mu\text{g/min/mg}$ protein, respectively. The relatively high V_{max} of the lung microsomes suggests that CPF exposed to the lungs via inhalation will be partially metabolized before entering the blood stream. The differing values of K_m for the lung and the liver suggest that different subsets of CYP450 enzymes are responsible for CPF metabolism in the lung than in the liver. Future studies will be used to investigate both TCP and CPF-oxon metabolism to provide further insight into the relative metabolic rates of TCP and CPF-oxon formation.

Sugars as Effective Scavengers to Reduce X-Ray Radiation Damage to Crystals

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X-ray crystallography is a technique used to determine the specific arrangement of atoms within a sample. The ability to obtain a high-resolution diffraction pattern is paramount for the construction of an accurate, detailed electron density map that translates into a comprehensive atomic structure. However, radiation damage is often a side effect of X-ray crystallography at second and third generation synchrotrons due to the inherent consequence of the interaction of X-ray photons with the atoms in the crystal. A scavenger molecule can be used to mitigate this damage by either co-crystallizing it with the protein or soaking it into the crystal after crystallization. The efficacy of several sugars as scavengers was evaluated. These sugars were co-crystallized with hen egg, white lysozyme. The affinity between the scavengers and the active pocket of lysozyme was simulated using Dr. David Ostrov's Molecular Docking program. The effect of the scavengers in the remediation or in delaying the onset of radiation damage was studied systematically at beam lines X6A and X4C at the National Synchrotron Light Source at Brookhaven National Lab. Currently, molecular replacement models are being calculated to determine the presence of the scavenger and to verify bond breakage, typically observed for radiation damage. This is an ongoing project that will require further data analysis.

Reduction of HOXA Gene Expression During Breast Cancer Progression

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Epigenetic changes underlie tumor progression and may lead to cancer specific expression of critical genes. We are interested in previous studies that have confirmed that the loss of expression of the HOXA gene cluster in human breast cancer is closely linked to aberrant DNA methylation. The HOXA genes are in the homeotic family, which encodes transcriptional regulators that play a critical role in the development and the differentiation of many multicellular organisms. Specifically HOXA1-HOXA11 are expressed in normal breast epithelium, but are epigenetically silenced in cancer cell lines. S1 cells were derived from HMT-355 cell of purified luminal epithelial cell population recovered from a breast biopsy of a woman with fibrocystic breast disease, and were found to be non-tumorigenic until grown in the absence of epidermal growth factor (EGF) for many passages which gave rise to tumors in nude mice. The cells cultures were then called T4-2 cells. T4-2 reversion (T4-TYR) was accomplished with the addition of tyrphostin, a pharmacological inhibitor of EGF which reverts malignant disorganized phenotype of the T4-2 cells in 3-D culture back to polarized structures. Microarray data and DNA methylation analysis have shown that HOXA2 and 5 genes are hypermethylated and silenced in T4 cells. Since all HOXA genes locate at the same gene locus, we proposed that the transcription of the whole gene locus is shut down because of the hypermethylation. Using an integrated approach of polymerase chain reaction (PCR) and quantitative real-time PCR (qPCR) we measured HOXA gene expression in S1, T4 and reverted T4 cells. The qPCR analysis confirmed the loss of HOXA gene expression in T4 cells. We also observed the expression levels of HOXA in the T4 reverted cells was comparably close to the HOXA expression in the T4 cells. This is an indication that the HOXA gene locus is silenced during breast cancer tumor progression due to DNA hypermethylation and that reverting the malignant phenotype in 3-D cultures has little effects on HOXA gene expression, indicating that DNA methylation at the HOXA gene locus is relatively stable, and that activity of HOXA is not required for the reversion.

Contemplation of the Reproductive Effects of Dioxins

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The chemical 2,3,7,8-Tetrachlorodibenzo-p-dioxin (TCDD) is one of the most toxic substances known to humans, hence one of the most widely studied environmental contaminants. It is a trace byproduct of many industrial processes, especially those involving combustion of organic compounds with small amounts of chloride and can be produced naturally by volcanoes, forest fires and burning vegetation, such as wood, in domestic stoves and fireplaces. TCDD causes a variety of adverse health effects including reproductive effects. Many people feel that there is no known safe level for dioxins. The manner in which one is exposed and the levels of exposure are significant factors in the risk. The purpose of this review is to provide an overview of dioxins' harmful effects through dose-response data on the reproductive system. One goal of the project was to construct a layout that could help identify the threshold for serious consequences of dioxin in the environment at various levels. The major toxic effects of TCDD on reproduction are decreased fertility, diminished ability to maintain a pregnancy, and possibly reproductive tract cancers. Relevant studies were identified through a computerized literature search of PubMed from 2000 to the present; the reference list abstract of retrieved articles was reviewed and then prioritized by level of relevance and key information. More than 450 articles on reproductive endpoints were reviewed and evaluated to identify key information for dioxin dose-response data and from those articles 109 were of high priorities. The aim was to reassess previous Environmental Protection Agency (EPA) risk assessments and compile and expand on current dose-response uncertainty information related to exposure and possible health effects of dioxin in order to respond to review comments from the National Academy of Science (NAS). Human exposure to environmental toxins cannot be avoided. Despite the abundance of studies surrounding this issue to better evaluate the risks towards humans, the relevance of such risk calls for further studies and a clear strategy to outline a clear and practical process for identifying and organizing studies.

A Computational Model for Analyzing the Biochemical Pathways of Matrix Metalloproteinase-2 (MMP-2) and MMP-9 in Collagen Type IV Proteolysis

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Cardiovascular disease is the leading cause of death in first world countries. The imbalance of matrix degrading enzymes and structural proteins within the extracellular matrix of an arterial wall is a critical factor in cardiovascular disease processes. Matrix metalloproteinase-2 (MMP-2) and matrix metalloproteinase-9 (MMP-9) degradation of collagen type IV results in migration and proliferation of vascular smooth muscle cells; this can lead to further narrowing of a diseased artery. Kinetic modeling of proteolysis is an approach which can be used to understand complex systems by describing the enzyme's mechanism and behavior quantitatively. In this research project, a computational model of biochemical pathways involved in activation and inhibition of MMP-2 and MMP-9 proteolysis of collagen type IV is being developed. Separate MMP-2 and MMP-9 models have been implemented within JSim, a software application developed by the University of Washington. Since MMP-2 and MMP-9 pathways overlap, the individual models will be integrated in the future. This MMP-2 model was also implemented in JDesigner, a tool of the Systems Biology Workbench, and DEVS, a discrete event system specification, for comparison of model environments. Various experimental methods for obtaining quantitative reaction rate parameters were explored, including high pressure liquid chromatography (HPLC) and fluorescence polarization. By pairing HPLC separation, largely by hydrophobic properties, with spectrometry techniques, protein and peptide identification and quantification is possible. Previous literature suggests the use of HPLC to measure enzymatic activity by using traces of the product/substrate itself as an internal standard. An experimental protocol for the measurement of the enzymatic activity of MMP-2 and MMP-9 is being developed. HPLC baseline standards for the individual substrates and enzymes are currently being measured and optimized. After baseline standards are determined the MMP enzymatic activity can be determined. The HPLC experimental results will be analyzed to derive the reaction rate parameters needed by the computational model. The use of HPLC methods to analyze the enzymatic activity of MMP-2 with collagen type IV and other correlated substrates provides parameters which cannot be obtained through literature. This research is in collaboration with the Vascular Research Laboratory at the University of Tennessee Medical Center in Knoxville.

Purification of Sumo-Tagged HBL-B, a Domain of a Pore-Forming Hemolysin Expressed in *Bacillus cereus*

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Hemolysin BL (HBL) is a unique pore-forming protein that has been observed in *Bacillus cereus*, an aerobic bacterium capable of causing food poisoning. In order to explore how HBL (along with its binding and lytic components) creates these pores and causes hemolysis, it needs to undergo a process of effective purification; this allows for a crystallization setup, the determination of the oligomeric protein structure, and the exploration of protein-cell membrane interaction. *Escherichia coli* cells containing a plasmid with binding component of HBL (HBL-B) gene (hblA), along with a sumo-tag (120aa peptide) followed by H6-tag were grown in a cell growing medium over a 48-hour time period. The cells were separated through centrifugation and lysed with suitable buffer (phosphate buffer, pH 8.0) and sonication. The protein, along with other soluble materials, was collected after ultracentrifugation of the lysed cells. The protein was purified using Ni-affinity chromatography and expression was confirmed using gel electrophoresis. This was then dialyzed over a 48-hour period along with a sumo-protease enzyme to cleave and remove the sumo tag. Because the HBL-B was not folding correctly (even with the sumo tag), the sumo-protease enzyme was ineffective and purification of the untagged protein was unsuccessful. Once the protein is successfully purified, a crystallization setup will follow, along with electron microscopy studies. The pore-forming mechanism of HBL-B will be studied using these results.

Development of a Yeast (*Saccharomyces cerevisiae*) System for the Discovery of p53 Response Elements in the Human Genome

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The p53 protein is a tetrameric transcription factor that acts as a tumor suppressor in mammalian cells. Upon induction, after genotoxic or non-genotoxic stress, the p53 protein binds to its specific response elements, and via transcriptional activation or transcriptional repression, induces DNA repair, cell cycle arrest, senescence or apoptosis, in a dose and cell-type, dependent manner. This project seeks to isolate functional DNA binding sites occupied by p53 in normal human fibroblasts after radiation exposure using an approach that combines

ChIP (Chromatin Immunoprecipitation) with a yeast-based screen for transcriptional activation. Locating and understanding the p53 target sites in the human genome is important for understanding its tumor suppressor function. A library of human DNA fragments, isolated by ChIP and cloned upstream of a yeast reporter gene, was screened in *S. cerevisiae* to identify those fragments able to confer transcriptional activation of HIS3 reporter gene. A total of 2.73×10^5 *S. cerevisiae* transformants containing a library plasmid and a p53 expression plasmid were screened for HIS3 reporter gene activation, using positive selection for growth on medium lacking histidine. Seven hundred sixty-two candidates were found to have the reporter gene activated in a p53 dependent manner. These candidates grew on medium without histidine only in the presence of p53. Small scale sequencing was done and a total of 36 non-redundant human DNA fragments were identified. A bioinformatics approach, used to match those fragments to the human genome, revealed a majority of them mapped at or near genes involved in cellular metabolism, signal transduction, or cancer development. These findings remain to be validated and further analyzed. This work is a part of a broader project that seeks to analyze the p53 function as transcription factor.

Seasonal and Cultivar Variation in Soil Organic Carbon of Soil Cultivated with Switchgrass at Milan, TN

Melissa Payton (CALIFORNIA STATE UNIVERSITY-FRESNO, FRESNO, CA 93728), Julie Jastrow (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). An increase in greenhouse gases, like carbon dioxide, has prompted the development of the Department of Energy's Consortium for Research on Enhancing Carbon Sequestration in Terrestrial Ecosystems (CSITE). This research focuses on studying how atmospheric carbon can be reduced through carbon sequestration in terrestrial ecosystems cultivated with the bioenergy crop, *Panicum virgatum* (switchgrass). While the above ground biomass of switchgrass may be used as biofuel, the below ground biomass may sequester carbon in the soil. Soil organic carbon (SOC) sequestered by switchgrass varies at different times of the year. The purpose of this study is to determine the seasonal and cultivar variation of soil organic carbon (SOC) in soil cultivated with switchgrass. Soil samples from four switchgrass cultivars during April 2008 were fractionated according to particulate organic matter (POM) >250 μm , POM >53 μm , silt and clay using wet sieving and centrifuging. Nitrogen and carbon percentages were measured for April 2008, at 0–5 cm and 5–10 cm depths, utilizing automated carbon and nitrogen analyzers. The overall trend revealed by the results shows an increase in SOC for the cultivars from April 2007 to April 2008 in the POM and silt fractions. Furthermore, the seasonal variation results reveal a decrease of SOC from April to July, an increase from July to October and an increase from October to April. The results indicate that carbon sequestration may be occurring in soil cultivated with switchgrass, and the amount of SOC varies depending upon season and cultivar. Future research needs to focus on determining the role soil microaggregates play in storing carbon.

Purification and Characterization of Recombinant *Aequorea coerulescens* Green Fluorescent Protein from *Escherichia coli*

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Green Fluorescent Protein (GFP) is a single chain polypeptide that forms a fluorescent chromophore by rapid cyclization and subsequent oxidation of residues Ser65, Tyr66 and Gly67. It is widely used as a fluorescent tag for in vivo investigations. In this study an efficient procedure was developed for the isolation and characterization of enhanced recombinant *Aequorea coerulescens* GFP (aceGFP) that was over-expressed in *Escherichia coli* JM109. The first step employed a three-phase partitioning to precipitate GFP using ammonium sulfate and tert-butanol. This was followed by dialysis and anion exchange chromatography. The purification procedure was monitored by UV/Visible absorption spectrophotometry, circular dichroism spectroscopy, fluorescence excitation/emission and sodium dodecyl sulfate (SDS) and native polyacrylamide gel electrophoresis (PAGE). Interestingly, two variants of GFP separated during anion exchange chromatography. The first variant (GFP478) absorbed maximally at 478 nm with a fluorescence emission maximum of 505 nm. The yield was 3.04 mg GFP478/g cell paste. The second variant (GFP493) had a maximum absorbance at 493nm and an emission maximum of 509 nm. The yield of this protein was 11.4 mg GFP493/g cell paste. Comparison of the UV/Visible and circular dichroism absorption spectra of the two isoforms indicate that the environments of their chromophores are different. Denaturing SDS-PAGE demonstrated that the lengths of their polypeptide chains are identical; however GFP493 migrated less than GFP478 by native PAGE, indicating a difference in the tertiary/quaternary structural characteristics of the two isoforms. GFP has been

successfully purified from recombinant *E. coli* in good yield, and the two resulting isoforms of aceGFP have been characterized. Small angle X-ray scattering will be used to further investigate the structural properties of these two proteins in solution.

Assessing Biogeochemical Activity in the Subsurface

Heather Poppen (WHITWORTH UNIVERSITY, SPOKANE, WA 99251), David W. Reed (IDAHO NATIONAL LABORATORY, IDAHO FALLS, ID 83415). Biomarkers can serve as indicators of change in the activity of microorganisms in response to a contaminant. Messenger RNA (mRNA) transcripts of functional genes represent a promising class of biomarkers for observing real-time biogeochemical activity in the environment. We are evaluating mRNA and DNA biomarkers for monitoring subsurface urea hydrolysis which plays a critical role in a remediation scheme for divalent trace metals or radionuclides in groundwater. Increased alkalinity due to the hydrolysis of urea by the native microbial population can lead to precipitation of calcite and coprecipitation of the trace metal, immobilizing the contaminant. The potential for this approach to sequester metal and radionuclide contaminants has been under investigation by the Idaho National Laboratory (INL) and collaborators for several years. The ureC gene (coding for the catalytic subunit of urease) and its mRNA transcripts are being investigated as biomarkers for subsurface ureolytic activity. One goal is to examine the correlations between the rate of urea hydrolysis and the levels of urease genes and mRNA transcripts in subsurface environments. We have collected biomarker samples from a field experiment conducted at the INL Vadose Zone Research Park, where molasses was used to stimulate the microbial community in a perched water zone and was followed by the addition of urea. Cells from 40-L volumes of water were collected on membrane filters using tripod filtration devices and were immediately frozen or treated with RNA^{later}® and returned to the lab for storage. Water samples were also collected for cell enumeration using the Acridine Orange Direct Count method. Results show an increase in cell number following amendment addition, indicating that the additions successfully stimulated microbial growth. Examination of cell count samples following the addition of urea showed possible evidence of calcite precipitation, suggesting that the urea addition led to enhanced calcite precipitation. Analyses by others indicate that an increase in microbial ureolytic activity occurred following amendment addition. Future work includes confirming the presence of calcite and implementing the developed extraction method to recover DNA and RNA. The latter will be used to examine the relationship between the levels of urease gene copies and mRNA transcripts and rates of urea hydrolysis, thus linking molecular biomarkers to biogeochemical processes.

Comparison Between Control and X-Ray Microbeam Irradiated HMECs with Total P53 and TP53^{ser15P}

Carolyn Posey (CREIGHTON UNIVERSITY, OMAHA, NE 68178), Eleanor Blakely (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). Breast cancer is the most common cancer among women, resulting in nearly 40000 deaths per year in the United States. While many factors contribute to the development of breast cancer, recent interest has focused on the effects of low-dose radiation on Human Mammary Epithelial Cells (HMECs). Many methods for investigation of the potential risk of radiation to HMECs rely on DNA damage-response markers, such as γH2AX , 53BP1 and TP53. In this paper we investigate the response of two HMEC lines to low doses, 50 or 100 cGy of 12.5 keV microbeam X-rays at 4, 7 and 11 μm widths. Previous studies in the Blakely group have shown HMECs in the stripe of dose responding with intense uneven fluorescence intensity to TP53^{ser15P}. Since the cells are asynchronous populations it was postulated that the uneven response may be due to cell cycle and/or density effects. S phase cells were labeled with EdU and studied and ruled out as preferentially labeling with TP53^{ser15P} or γH2AX ^{ser139}. The Total P53 response of the two HMEC cells under investigation, with or without radiation, had not been studied to date. Unirradiated fields of S1 cells showed Total P53 signal in almost every cell; however the cells did not have identical fluorescence intensity. We will show the distribution of intensity of Total P53 in irradiated and unirradiated fields, compared to the distribution of intensity for TP53^{ser15P}. We will also show that cells can be labeled with optimal intensity and sharpness with γH2AX ^{ser139} (to clarify the pathway of the X-ray microbeam) and observe the characteristic whole nuclear TP53^{ser15P} response in the same cell, to show if a cell hit in the cytoplasm or what portion of the nuclear volume must be hit to initiate a TP53^{ser15P} response.

Polymeric Micelles as Probes for In Vivo Fluorescent Imaging

Chyara Rivera (UNIVERSITY OF PUERTO RICO-MAYAGÜEZ, MAYAGÜEZ, PR 00680), Hao Chen (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). Amphiphilic polymers assemble into nanoscopic supramolecular

structures, termed polymeric micelles, which are under extensive study for drug delivery. There are several reasons for this growing interest. Polymeric micelles poorly solubilize water-soluble drugs and have a long circulation time in blood as compared with other types of delivery systems. These vesicles are promising candidates for the next generation of drug carriers with targeted and controllable drug release. In this project we explore the use of dye loaded polymer micelles as imaging probes for disease diagnosis. From block copolymer of poly(caprolactones)-b-poly(ethylene oxide), 45 target-specific polymeric micelles loaded with fluorescence dye molecules in their hydrophobic cores were made. The objective of the project is to characterize the better dye that gives the best fluorescence signal suitable for in vivo imaging. The dye with the best fluorescence signal in solution and encapsulated in the micelle was SQII. SQII is expected to be used as a probe to track tumors in the body.

Glowing Gonads: A Study of Meiosis in *Caenorhabditis elegans*

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The preliminary stages of meiosis, the development of gametes, have a critical role in the longevity of a population. Research using *Caenorhabditis elegans*, a model organism when studying meiosis and cellular development, may provide researchers the clues to reproduction and development in other more complex organisms like humans. Here we address two projects related to meiosis. Project 1 involves finding the phenotype of the unknown meiotic mutant, JA32, and Project 2 focuses on making pairing center proteins, him-8 and zim-3, expression clones. Phenotypic data of the JA32 strain (Project 1) was gathered by means of immunofluorescence staining with antibodies for the pairing center protein HIM-8. Pairing center proteins such as HIM-8 have a fundamental function in the pairing of homologous chromosomes. The immunofluorescence images indicate the JA32 strain lacks a transition zone, the region where pairing of homologues occur, indicating a pairing defect. JA32 has multiple HIM-8 foci in pachytene that suggest the X-chromosome is not pairing. The presence of >6 diaminido-2-phenylindole (DAPI) staining bodies at diakinesis in JA32 is expected of a pairing defect and indicates the autosomal chromosomes may possess a recombination defect. In the construction of the pairing center expression clones (Project 2), the genes, zim-3 and him-8 and corresponding 3' UTR regions have been amplified and purified successfully. Zim-3 and him-8 code for the pairing center proteins that aid in the pairing of homologous chromosomes. The purpose of the expression clones for use in a future immunoprecipitation (IP) experiment to find out how these pairing center proteins interact with other structures in the membrane.

Characterizing Putative Liver Enhancers in the Frog *Xenopus tropicalis*

Cai Roberts (UNIVERSITY OF CALIFORNIA—DAVIS, DAVIS, CA 95616), Gabriela Loots (LAWRENCE LIVERMORE NATIONAL LABORATORY, LIVERMORE, CA 94550). Vast stretches of the genome do not code for protein products; rather, leading theory suggests that some may serve as regulatory sequences for neighboring genes. Not much is known about how these sequences function to control gene expression or how to distinguish them from nonfunctional DNA. This study analyzes the possibility of tissue specificity of gene enhancement in *Xenopus tropicalis*. Bioinformatics techniques were applied to identify stretches of DNA that are highly conserved between species, yet did not appear to have any coding function. These sequences were ranked based on their potential to regulate gene expression in the liver. Once identified, these sequences were cloned and ligated into a plasmid vector containing a red fluorescent reporter gene, Katushka. The vector also contains *Tol2* transposable element arms, one on either side of the cloned region, to allow for efficient integration into the frog genome. Transgenic constructs were injected in *Xenopus* at the single-cell embryonic stage to allow for in vivo characterization of these putative enhancer elements and to determine whether they are able to enhance reporter gene expression. Based on results from similar experiments, one out of three predicted sequences should indeed be a liver enhancer element. At present, one construct has been shown to be a liver enhancer, and in vivo studies to confirm the one-third success rate are still underway. Further studies of enhancer activity will improve understanding of genome architecture and function and how these relate to susceptibility to disease.

The Comparison of Conventional and Emulsion Polymerase Chain Reaction for Detecting Less Concentrated Vaccinia DNA

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In medical diagnostics, low concentrated viral DNA can easily go undetected, and physicians may be unable to determine the cause of viral symptoms. In a medical sample, highly-concentrated DNA tends to dominate the polymerase chain reaction (PCR) reagents for replication. Conventional PCR is the repetition of thermal cycles that amplify an aqueous reaction consisting of DNA and PCR reagents. Without access to the PCR reagents, the less concentrated viruses will not show up on an electrophoresed gel where DNA separates and appears as bands. Theoretically, unlike conventional PCR, emulsion PCR has the ability to detect a single copy of target DNA. In emulsion PCR, DNA is separated into picoliter aqueous droplets cloaked in oil. When isolated from the highly-concentrated DNA, the less concentrated DNA should have better access to the PCR reagents and replicate better. To test the effectiveness of emulsion PCR, a multiplex (simultaneous amplification of two or more DNA templates) was done on vaccinia virus (VV) and lambda (λ) DNA through conventional PCR and emulsion PCR. The VV DNA was instituted as the minority with a constant concentration of 1×10^4 copies; the concentration of λ DNA varied from 1×10^4 to 1×10^9 copies. It was predicted that conventional PCR would produce only the dominant λ DNA, and emulsion PCR would produce both λ DNA and VV. However, these experiments oppose this prediction. Several experiments support that conventional PCR is substantially more reliable. Conventional PCR repeatedly produced both amplicons even when at vastly contrasting concentrations (VV at 1×10^1 and λ at 1×10^9 copies). Emulsion PCR, in contrast, only produced the λ amplicons. The aqueous reaction in the picoliter droplets did not contain all the essential reagents for replication. This project did not have access to technology capable of creating uniform droplets containing every reagent. Overall, emulsion PCR is substantially more time-consuming and unreliable for multiplexing. These experiments support the use of conventional PCR over emulsion PCR when simultaneously detecting viral DNA.

Expression, Purification and Preliminary Characterization of GamC, A Protein Required for *Salmonella enterica* Serovar Typhimurium Virulence

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An estimated 1.4 million cases of *Salmonella* infection occur annually in the United States, and about 400 of these are fatal. *Salmonella enterica* serovar Typhimurium (STM) is among the most common strain of *Salmonella* serovar causing Salmonellosis in the U.S. STM infections are also believed to be at least thirty-fold underreported, with millions of cases occurring every year. GamC is a novel protein required for STM survival within host macrophages and for STM virulence. It is located within an operon whose putative function is involved in mediating macrophage colonization allowing for the establishment of systemic infections. The goal of the project is to express, purify and characterize GamC. The purification and isolation of GamC involved expression of the protein in *Escherichia coli*, followed by purification via a nickel column and size exclusion chromatography. SDS-PAGE and Western Blots were used to determine purity. To determine activity, a colorimetric acetyl-CoA assay was utilized. GamC was purified to ~90% purity with a final yield of about 25 μ g/L. Preliminary functional characterization data suggests that GamC functions as an acetyl-CoA hydrolase producing acetate, which can be involved in alteration of the peptidoglycan layer of the bacterial cell wall allowing for reduced susceptibility to macrophages. The purified GamC will enable structural studies towards the development of a small molecule (pharmaceutical drug) to inhibit the activity of a protein required for *Salmonella* virulence.

Contribution of Autotrophic and Heterotrophic Respiration to Soil Respiration

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As global warming becomes a major issue throughout the world, understanding how carbon dioxide (CO_2) is exchanged through the atmosphere and biosphere is of the utmost importance. This project was part of the Ameriflux Program, which seeks to understand factors driving soil carbon storage and net ecosystem exchange of carbon in different ecosystems in North America. The program consists of 120 field sites across the United States, and this project's site was located at Fermilab National Accelerator Laboratory in Batavia, IL. The site was located on an 18-year-old restored prairie that previously had been used to cultivate a corn and soybean rotation for over 100 years. The main goal of this project was to distinguish between heterotrophic and autotrophic CO_2 respiration from the total flux and to determine how the

variance of abiotic (soil temperature and moisture) factors affect short-term ecosystem respiration. At this site, CO₂ levels respired from the soil were measured around the site using an infrared gas analyzer. Soil respired gas samples were also collected in 100-mL evacuated flasks at concentrations varying between 400 and 700 ppm from the same areas in order to calculate the d13C (ratio of ¹³C/¹²C) of soil respired CO₂ by implementing Keeling plots. Soil cores were also extracted up to 15 cm deep as a means for measuring the d13C of respired CO₂ from both the roots and microbial community. This information provides insight into the fraction of respired CO₂ that comes from heterotrophic and autotrophic components and to identifying how abiotic factors, such as soil temperature and moisture, affect soil respiration, auto and heterotrophic respiration in a grassland ecosystem. Results showed that soil moisture and temperature had no effect on either heterotrophic or autotrophic respiration. Further research needs to be done in order to understand the factors driving soil respiration, the central path for carbon traveling through terrestrial ecosystems and into the atmosphere. Understanding this process could play an important role in the mitigation of global warming.

Clumping by *Desulfovibrio vulgaris* Hildenborough

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Desulfovibrio vulgaris Hildenborough is a ubiquitous sulfate-reducing bacterium with great potentials in bioremediation. Clumping, a likely precursor of biofilm formation, was observed in wild-type *D. vulgaris* cultures when cell densities reached approximately 108 cells/ml. *D. vulgaris* cultures without the ~200-kb plasmid showed a decreased clumping ability. To understand the differences between these two strains, both wild-type and plasmid-less strains were grown anaerobically in 5-liter bioreactors in batch mode and samples taken every five hours. Growth of the organism was monitored by continuous bioreactor parameters data logging (i.e., optical density, pH, temperature, mixing and redox potential) and live/dead differentiation staining. The wild-type strain grew slower than the plasmid-less strain and produced less biomass by the time stationary phase was reached. Whole-cell fatty acid methyl ester (FAME) analysis and real-time PCR were performed on every sample. Clumping progression was also imaged by scanning electron microscopy (SEM). Images showed significant differences between the two strains in surface structures and extracellular material(s). These results suggest that genes located on the plasmid may have effected growth and clumping.

Photosystem I for Artificial Sight (Standardization of PSI Isolation by Hydroxylapatite Chromatography and Incorporation into Liposomes)

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Macular degeneration is a progressive disease that destroys the photoreceptors in the eye resulting in a loss of perception of light. It affects approximately 13 million people in the United States. Performing a similar function to the photoreceptors in the eye, a photosynthetic protein complex in plants called Photosystem I (PSI) carries out electron conduction activated by visible light. If PSI is incorporated successfully into retinal cells in eyes, light sensitivity can be restored by replacing the inactive photoreceptors. Previous research has shown that PSI can be incorporated into mammalian cells using liposomes as transport vesicles. In order to test the PSI liposome's reaction to a solution more similar to cell fluids, we incorporated the proteins into liposomes using a buffer with higher NaCl concentrations than the previously used Tris-HCl based buffer. The liposomes were not damaged by the physiological saline solution. Using hydroxylapatite chromatography PSI was isolated from chloroplast membranes. We measured PSI activity of four different species: Bloomsdale-like spinach, baby spinach, wheat grass and duckweed. Wheat grass (*Triticum aestivum*) had the most PSI activity per chlorophyll mass (34.3 mV/mg chlorophyll). This species also germinated readily and grew rapidly under laboratory conditions. These studies will enable the eventual production of standardized liposome vesicles containing Photosystem I for future therapeutic treatment of patients blinded by macular degeneration.

Using Dynamic Light Scattering for Membrane Protein Studies in the Hyperthermophilic Archaeon *Sulfolobus solfataricus*

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The hyperthermophilic archaeon *Sulfolobus solfataricus* lives in nearly boiling, acidic waters of geothermal hot springs around the world. Hyperthermophiles offer the advantages of studying transient protein complexes that may be more stable at room temperature, allowing for

the study of otherwise short-lived complexes. Furthermore, it is widely accepted that Archaea are more closely related to Eukarya (humans) than to Eubacteria. The work presented here is preliminary to isolating and characterizing membrane bound proteins of *S. solfataricus*. *Sulfolobus* cells were lysed using the French Pressure cell press to produce inverted membrane vesicles (IMVs). Ultracentrifugation and Fast Protein Liquid Chromatography (FPLC) were used to separate cell components according to size and identify the IMV-rich fraction. Serial dilutions of an IMV-rich fraction were used to determine an appropriate concentration for analysis with dynamic light scattering (DLS). IMVs were screened with detergents that were selected for their ability to lyse the IMVs and therefore release membrane proteins for further characterization. The detergent DDMAB was investigated for the ability to solubilize and isolate membrane bound proteins from the IMVs. Results show that at 40% of the critical micelle concentration (CMC), DDMAB appears to disrupt IMV structure. Therefore the results suggest a detergent concentration in this range may be utilized for IMV membrane protein isolation. Further studies are needed to obtain pure protein isolates for future characterization with SAXS (small angle X-ray scattering). This work is part of the Molecular Assemblies, Genes and Genomics Integrated Efficiently project (MAGGIE) which is a component of a larger DOE program known as Genomes to Life (GTL). MAGGIE is combining information from three genera of Archaea (*Pyrococcus*, *Sulfolobus*, *Halobacterium*) using mass spectrometry, SAXS and bioinformatics, the major goal being to characterize the complexity of protein interactions in living systems. Major possible applications include: bioenergy production, environmental remediation and carbon sequestration.

Transcriptional Regulation of Sclerostin in Van Buchem Disease

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Sclerostin (SOST) is expressed in osteocytes and has been identified as a negative regulator of bone growth. SOST is a key regulator in bone formation, and the lack of SOST results in progressive bone overgrowth, a disease called Sclerosteosis. Sclerosteosis is a disease similar to Van Buchem disease, and both show a phenotype of bone overgrowth. Van Buchem disease is associated with a 52 kilobase (kb) deletion, which is only 32kb downstream of the SOST gene. A putative bone enhancer, ECR5 (Evolutionarily Conserved Non-coding Region) was identified between SOST and the downstream gene MEOX1, found inside the Van Buchem deletion region. ECR5 has been shown to drive bone-specific expression of a reporter gene, luciferase, in cell culture, and was identified as a promising bone enhancer element. This study focuses on the expression pattern of ECR5 in vivo, to recapitulate part of the endogenous SOST expression as examined by LacZ stain. LacZ is a promoter construct and is expressed where the enhancer ECR5 is driving it. Other mouse lines such as the myocyte enhancer factor 2 (MEF2) may be interacting with SOST expression. Mef2C is an identified transcription factor that was found in the SOST bone enhancer. The study also explores the characterization of related mouse lines, such as MEF DMP-1 and MEF COL-1 that may reveal genetic interactions with SOST in vivo. Transgenic mice carrying the ECR5 enhancer and a minimal promoter (mouse beta-globin) driving beta-galactosidase or LacZ reporter gene expression were generated. After dissection and decalcification, LacZ stains were done on ECR5L-LacZ and SOST KO-B transgenic mice embryos, 10.5–14.5 days old, and on the long bones and calvaria of SOST KO-B, ECR5L, MEFDMP-1 and MEF COL-1 mice. Samples were then photographed for observation and some were embedded, sectioned into slides and counterstained. This experiment shows that that ECR5 is in fact expressed in ECR5L-LacZ transgenic mice. It also suggests that ECR5 is fully dependent of Mef2C because there is no expression in the osteocytes, when Mef2C is conditionally inactivated in both osteoblasts and osteocytes.

Structural Studies of Light Harvesting Complex II

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With the increasing economic and political implications of using fossil fuels, the need for the creation of alternate energy sources has become a necessity. Solar energy, being the most abundant and non exhaustible source of energy, is one of the leading areas in alternate energy research. Light harvesting complex II (LHCII) is the major chlorophyll binding protein found in the thylakoid membranes of plants and is responsible for the light harvesting and structural properties of the photosynthetic membrane. We are investigating the properties of LHCII in order to better understand its structure, assembly in the photosynthetic membrane and light harvesting/exciton diffusion

properties. Two procedures were used to obtain LHCII. In both, we purified LHCII from fresh spinach leaves by extracting and lysing the chloroplasts, followed by solubilizing the thylakoid membranes with detergent. In the first procedure, we appressed the LHCII using Mg^{2+} and K^+ salts, followed by a centrifugation over a 0.5 M sucrose cushion to separate LHC II from other solubilized thylakoid components. In the second procedure, a gradient density centrifugation step (0.1 M to 1 M sucrose) was introduced, before the appression step, to separate LHCII from larger solubilized membrane components. In previously published literature, pure LHCII has a chlorophyll a to chlorophyll b ratio of less than 1.3. By comparison of the chlorophyll a to chlorophyll b ratio in LHCII, we determined that the second procedure resulted in a purer preparation of the protein. The Chlorophyll a to Chlorophyll b ratio was 1.79 in the first procedure and 1.28 in the second. The yield and purity were also more consistent using the second procedure. Circular dichroism spectroscopy and small angle neutron scattering were used to study the structure of LHCII in the β -octyl-glucoside (BOG) solution. Purified LHCII was dissolved in BOG solution at 45:1 detergent to chlorophyll ratio with the chlorophyll concentration at 1.22 mg/ml. The radius of gyration (Rg) of the LHCII preparation was determined to be 26.3 ± 2.8 Å. This is consistent with previously published crystal structure of LHCII trimer which has a Rg of 27.9 Å. The data shows that LHCII remained intact in a detergent solution for an extended period of time. This data will significantly help future research in determining how LHCII interacts and stays intact in novel synthetic polymer membrane systems.

High-Throughput Protein Purification and Crystallization for Structural Genomics

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The three-dimensional atomic structure of proteins will help elucidate targeted biochemical functions. Argonne National Laboratory (ANL) is collaborating with the Midwest Center for Structural Genomics (MCSG) to identify the best conditions for increasing protein solubility to generate a higher yield of crystal production, which leads to rapid and affordable protein structures. MCSG is inducing recombinant proteins in *Escherichia coli* under different conditions to optimize protein expression and solubility. For the purification process, MCSG is using two rounds of immobilized metal-ion affinity chromatography (IMAC). The protocol has been implemented by using AKTA EXPRESS, which is capable of performing multidimensional chromatography. The second project involves collaboration with the Center for Structural Genomics of Infectious Diseases (CSGID) to clone targeted proteins from pathogens in the National Institute of Allergies and Infectious Diseases (NIAID) Category A-C priority lists. The current goal of CSGID is to establish a protocol for optimizing a genetically enhanced *E. coli* strain (Magic BL21) to accept a wide range of BioSafety Level 2 (BSL2) bacterial and eukaryotic vectors. Eventually, a protocol for high-throughput (HTP) purification and crystallization of targeted proteins will be created for organisms that cause current and ongoing infectious diseases. The process of purification and cloning is vital for the investigation of atomic structure of proteins. The results of the projects will yield insight into the target molecular mechanisms, thereby elucidating protein function, which will lead to improvement in future drug designs and disease treatments.

Testing of Low-Cost Samplers for Collection of Particulate Matter From Second Hand Smoke

Erik Spickard (UNIVERSITY OF CALIFORNIA—DAVIS, DAVIS, CA 95616), Lara Gundel (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). A low-cost compact sampler with the ability to collect gas and particulate matter (PM) over three separate areas is being developed to enable epidemiologists to do large scale studies of exposure to secondhand smoke (SHS). This research focused on characterizing the operation and collection efficiency of the PM sampler and assessing the equivalence of the three deposition areas. Various tests were done: one test was in an open building to sample ambient wood smoke and the other tests were in an SHS test chamber with samplers rotating collection areas every 8 hours, every 5 minutes, not rotating and not rotating with two samplers in series. Some tests were done with no PM source to determine sources of error and related uncertainty in sampler durability, measurement methods and measurement equipment. Collection of PM was assessed by measuring the absorbance of light passing through the sample area. The ability to get desired results improved as testing progressed. The first test had almost no useable data but identified a problem that was later solved. The SHS test chamber experiments with various time intervals gave expected results with improving agreement. Tests for sources of error showed that the

quartz components of the samplers needed caps to protect them during testing. This work concluded that the next important task for the project is to reconfigure the sampling equipment to reduce uncertainty and improve precision, and then to repeat select experiments to confirm collection efficiency.

Characterization of DNA Immobilization and Hybridization on Piezoresistive Microcantilever Surfaces

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Rapid and efficient detection of DNA hybridization is an essential concept in designing genomic-based diagnostic tests. Most current methods employed in detecting DNA hybridization require a fluorescently or radioactively tagged known DNA sequence, a time consuming and costly process. Microcantilevers provide an ideal surface for immobilizing and hybridizing DNA without relying on labeling but instead utilizing the change in surface stress induced by the chemical interactions. Although many studies have illustrated DNA immobilization and hybridization on cantilever surfaces, there still remains much to be gained by characterizing optimal conditions for these interactions. The aim of this work was to characterize DNA hybridization and immobilization at varying temperatures and flow rates in an effort to discern the optimal conditions for such reactions. Microcantilever arrays consisting of four piezoresistive cantilevers were coated with gold and then introduced into the CantiLab4 flow system equipped with a Peltier-based heating cell. DNA immobilization on the cantilever surface was achieved by injecting thiolated ssDNA into the flow system. These cantilever arrays were then used to detect hybridization of the complementary strand at varying temperatures using the Peltier cell to achieve a steady temperature. Both immobilization and hybridization experiments were conducted under flow and static conditions. Preliminary results suggest that flow conditions produce a stronger immobilization signal than that of static conditions. DNA immobilization conducted under flow conditions also exhibits a change in noise level after DNA immobilization. This study provides preliminary results that may aid in designing a genomic diagnostic testing device with a flow system for use in the health-care field.

Ion Trap Mass Spectrometry Evaluation of Solvents Used for Mobile Phases in High-Throughput Proteomics Laboratory

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The effectiveness of electrospray ionization mass spectrometry (ESI-MS), a widely used analytical technique for proteins and peptides, depends upon its sensitivity and detection limit. Background ions detected in the spectra can interfere with quality mass spectrometric analysis of proteins and peptides. In this study, various permutations of the solvents used as mobile phases for the mass spectrometry instruments — using solvent components obtained from different sources — were tested in order to determine whether changing the solvents to another source from the one currently used would minimize the current spectral background. Aqueous, organic and formic solvents were prepared using three sources of acetonitrile (Optima, Optima LC-MS, LC-MS from Burdick & Jackson) and four sources of water (laboratory nanopure, OmniSolv, Burdick & Jackson and sample water from Burdick & Jackson); two pre-made formic solvents were tested as well. Infusion lines were prepared with brand-new syringes, with one syringe set-up for the aqueous solvents and another for the organic solvents. Samples were directly infused into the instruments, and ten scans were collected per data set. From the spectra collected, peaks of interest noted included: a large 550 m/z peak, 445 m/z and 391 m/z. Based on tables of common ESI background ions published by solvent manufacturers, the 550 m/z peak was attributed to new syringe plungers; a confirmation test was performed using an older, used syringe, and the relative intensity of the peak decreased. The 445 m/z ion was attributed to polysiloxanes, and the 371 m/z was due to plasticizers. It was determined, based on the spectra collected for each solvent, that the lab solvents currently in use are acceptable in comparison to those prepared with the purchased components and more cost-effective for the lab. These solvents could be tested using a high-resolution instrument or performed on a column to obtain confirmation and solid results.

Preliminary Crystal Structure Analysis of Proteins with Oxidoreductase Functions

Charlyn Thomas (MEDGAR EVERS COLLEGE, BROOKLYN, NY 11225), S. Swaminathan (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). The Protein Structure Initiative (PSI) is a NIH-sponsored project to determine the crystal structure of every protein family. As part of PSI,

the crystal structure determination of three oxidoreductases from *Agrobacterium tumefaciens*, *Salmonella typhimurium* and *Chlorobium tepidum* has been carried out. Hypothetical cloned proteins (target ID 11128a, 11128j and 11128k), from the above bacterial sources were obtained from the New York Structural Genomics Research Consortium (NYSGXRC). All three of these proteins are known to have oxidoreductase functions. The best diffracted crystals were obtained from 11128a, bacterial source *A. tumefaciens*, whose data is represented in this study. *A. tumefaciens*, a rod-shaped gram-negative soil bacterium, is the causal agent of Crown Gall disease (the formation of tumors in plants) in over 140 species of dicot, such as grapevines, stone fruits, nut trees, sugar beets, horseradish and rhubarb. This causes great concern for the agricultural industry. By crystallizing these proteins, the structure-function knowledge will be used to understand their malfunctions and possibly derive treatments. All three proteins were crystallized using the sitting drop method to determine their structures and active site behaviors. The crystals were obtained in the reservoir containing initial screens of polyethylene glycol (PEGs) suite and ammonium sulfate (AmSO_4) suite, and were later optimized for better results. The crystals were selected to collect X-ray diffraction data at beam line X12-C of the National Synchrotron Light Source at Brookhaven National Laboratory (NSLS, BNL). The data was collected using CBASS and was processed by utilizing the computer software, HKL2000. These proteins/enzymes are involved in the catalysis of oxidation-reduction (redox) reactions, which utilize nicotinamide adenine dinucleotide phosphate (NADP) and nicotinamide adenine dinucleotide (NAD) to perform their functions. The crystal structures will provide information about the enzyme's active sites and protein folding. By knowing the structure of this protein, attempts can be made by pharmaceuticals to limit its pathology in the agricultural industry.

Bioadhesives Production

Jeffrey Thurman (BRIGHAM YOUNG UNIVERSITY-IDAHO, REXBURG, ID 83440), Heather Silverman (IDAHO NATIONAL LABORATORY, IDAHO FALLS, ID 83415). Proteins isolated from the foot organ of *Mytilus edulis* (Blue Mussel) have been shown to have useful adhesive properties including water resistance, low toxicity and strength. It was necessary to obtain pure stocks of yeast cells (*Saccharomyces cerevisiae*) containing *M. edulis* foot proteins (Mefp 1, 2 or 3) for production of the recombinant bioadhesives. Stocks of yeast containing the recombinant Mefp proteins were analyzed. Polymerase chain reaction (PCR) and DNA sequencing were performed to confirm that the new Mefp-specific clone stocks were pure and retained the correct genes for the bioadhesive proteins of interest. Fresh stocks of *S. cerevisiae* containing Mefp clones were grown on SC Ura-medium (+2% Raffinose). Samples taken from prior purification processes were analyzed for concentration using a Bradford micro-assay and then separated by electrophoresis. Single-colony PCR assays with Mefp-gene-specific primers were conducted using conventional reaction parameters. The PCR products were analyzed for size on a 1.2% agarose gel, stained with ethidium bromide, and visualized with an AlphaImnotech imager. PCR products were purified using a Min-Elute column. DNA concentrations of purified products were tested using a Nanodrop spectrophotometer. DNA sequencing of PCR products was conducted using an ABI 3730 DNA Analyzer and the sequences were analyzed with NCBI BLAST tools. Results of colony growth for each Mefp protein were successful. Analysis of the electrophoresis gel showed amplicon sizes were as expected for the published Mefp clones: 1.698 kB (Mefp-1), 1.362 kB (Mefp-2), 1.413 kB (Mefp-2 clone 7) and 0.216 kB (Mefp-3). Analysis of the protein gel showed bands at expected size ranges for the recombinant Mefp proteins. BLAST analysis matched the published nucleotide sequences in GenBank. Purified PCR products contained sufficient DNA concentrations as to allow for continued experimentation. New colonies of Mefp will maintain a viable source for future PCR templates. Protein concentrations helped identify samples with sufficient quantities of desired proteins for use in future testing. PCR and DNA sequencing confirmed that Mefp-specific clone stocks for three bioadhesive proteins of interest — Mefp-1, -2 and -3 — are available for follow-up recombinant protein production studies. Continued work will focus on providing samples of purified recombinant bioadhesive proteins to interested partners for testing and production.

* Phosphoinositide 3-Kinase (PI3K) Inhibition via Apurinic/ Apyrimidinic Endonuclease-1/Redox Effector Factor-1 (Ape-1/Ref-1) Up-Regulation of the Protein Phosphatase and Tensin Homolog (PTEN)

Melissa Torres (STATE UNIVERSITY OF NEW YORK-STONY BROOK, STONY BROOK, NY 11970), Louis Peña (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

The goal of this project is to increase radiosensitivity of endothelial cells by targeting the cellular Ras/PI3K/Akt signaling pathway and to investigate whether APE-1/Ref-1 interacts with this pathway. Histone deacetylase inhibitors (HDI) may play a role in the APE-1/Ref-1 activation or deactivation, which may lead to up-regulation of PTEN. PTEN is a regulator of the PI3K pathway. When it is up-regulated, it causes an increase of apoptosis by inhibiting PIP3, a downstream product of PI3K. PTEN is regulated by early growth response protein-1 (Egr-1). The transcription of Egr-1 is activated by ionizing radiation. When Egr-1 is induced by ionizing radiation it is predicted that the up-regulation of PTEN will result in higher levels of apoptosis, which may cause the radiosensitization of endothelial cells. To explore these interactions, radiation induced apoptosis assays were performed using bovine aortic endothelial cells (BAEC), scriptaid fibroblast growth factor (bFGF) and basic bFGF. A titration experiment was done to obtain non-lethal concentration of scriptaid (an HDAC inhibitor) in endothelial cells in order to view the apoptotic effect of this inhibitor on endothelial cells. The most effective concentration was between 1–5 ug/ml of scriptaid. Other HDIs may be used, such as trichostatin A (TSA). A subsequent experiment was to use the HDAC inhibitor with and without bFGF (a growth factor that activates PI3K). Further experiments to explore this pathway will involve the inhibition of APE-1/Ref-1 by the small molecule CRT0044876 with and without the presence of bFGF. It is expected that there will be a decrease in apoptosis when APE-1/Ref-1 is inhibited by CRT0044876. Once these preliminary experiments are performed, we may then explore the PTEN activity when PTEN and APE-1/Ref-1 are both activated to further support the predicted cell signal transduction pathway. The radiosensitization of endothelial cells by the methods explained will help to target tumors in radiation therapies. One major area of interest surrounding this predicted pathway that should be explored by continuing researchers is the relationship between APE-1/Ref-1 activating P53, a transcription factor for PTEN. The project described here is ongoing research that is being continued by personnel in Dr. Peña's lab at Brookhaven National Laboratory.

Probing HIV Gene Regulation Using Noise Correlations

Tommy Trimeloni (MIAMI UNIVERSITY, OXFORD, OH 45056), Mike Simpson (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). We are developing a model for showing how gene expression regulation occurs in HIV to provide insight into possible therapeutic strategies. We ultimately aim to understand the information processing encoded in HIV genetic circuits that control post-infection development. The problem with defeating HIV, or any retrovirus, is that it can mutate quickly, which allows the virus to circumvent many therapeutic strategies. By gaining a detailed mechanistic understanding of the 'master program,' we hope to provide insights that lead to new therapeutic strategies. Human T-cells were infected with either a wild-type or a mutant full-length virus with a green fluorescent protein (GFP) reporter gene spliced in place of the negative-factor protein gene (Nef), or a minimal virus containing only a single gene for regulation and a GFP reporter gene. We tracked the infected T-cells over periods as long as 30 hours using time-lapse fluorescent microscopy at 10-minute intervals. We analyzed correlations in the noise of GFP expression as a novel means of probing the regulation of two genes that control the latent/active infection decision in HIV-infected cells. The two genes were tat (trans-activator of transcription) and rev (the regulator of expression of virion proteins). The measurement of the noise correlations provides a measure of the strength of positive autoregulation (feedback) in the circuit as the latent/active infection decision is being made. The measurement of noise correlation also provides information about the sequence of events that unfold during early infection. Tat is a positive regulator of its own expression and drives the circuit toward active infection; rev, in contrast, may provide negative regulation that switches the circuit into the later phase of viral development, which leads to active infection. In the case of the full-length virus, this switching event is marked by a sharp burst in gene expression clearly evident in the time-lapse fluorescence microscopy of GFP noise. Our analyses of the noise correlations at this switching point provide key insights for developing a more complete model of the gene-regulation strategy used by HIV to drive the infection forward.

Preliminary Neutron and Ultrahigh Resolution X-Ray Single Crystal Diffraction Studies of the Aspartic Proteinase Endothiapepsin Co-Crystallized with a Gem-Diol Inhibitor PD-135,040

Han-Fang Tuan (GRINNELL COLLEGE, GRINNELL, IA 50112), Leighton Coates (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Aspartic proteinases are a class of enzymes widely distributed among fungi, plants, vertebrates and viruses. They are involved in numerous disease conditions, including hypertension, amyloid disease, malaria and AIDS. Aspartic proteinase inhibitors have a proven therapeutic

effect in the treatment of AIDS. The aspartic proteinase class of enzyme is comprised of two structurally similar domains, each contributing an aspartic acid residue to form a catalytic dyad that cleaves the substrate peptide bond. The enzyme used in these studies is endothiapepsin, a member of the aspartic proteinase family, which is composed of 330 amino acid residues, with roughly 170 residues in each domain. The crystallographic studies of the catalytic mechanism of aspartic proteinases have largely been done on enzyme-inhibitor complexes that mimic the putative transition-state intermediates. The gem-diol class of inhibitors mimic both of the hydroxyl groups that are thought to exist in the transition-state. In this study, endothiapepsin has been co-crystallized with a gem-diol inhibitor PD-135040 in a low solvent content unit cell (39%), which is unprecedented for this enzyme-inhibitor complex. This enables atomic resolution (1.0Å) X-ray single crystal diffraction data to be collected at 100K on beamline ID14-2 at the European Synchrotron Radiation Facility (ESRF). Bond length analysis from this atomic resolution X-ray data set was used to deduce the protonation states of the two catalytic aspartates. Results show that one aspartate, Asp215, is protonated on the outer oxygen while the other aspartate, Asp32, is negatively charged when the inhibitor is bound. A room temperature (298K) X-ray single crystal diffraction data set was collected on an in house rotating anode X-ray generator. A room temperature (298K) neutron single crystal diffraction data set was collected at the Protein crystallography station (PCS) beamline at the Los Alamos Neutron Science Center (LANSCE) spallation neutron source. These data sets will be used for joint X-ray/neutron refinement to visualize the hydrogen/deuterium atoms at the active site. Through locating the catalytic hydrogen atoms in this complex, we will get a clearer understanding of the catalytic mechanism of aspartic proteinases.

Protein Purification for Structural Genomics

Jessica Vela (UNIVERSITY OF TEXAS—PAN AMERICAN, EDINBURG, TX 78541), Rachele Hendricks (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). The primary objective of the Structural Genomics Program at Argonne National Laboratory is to determine the three-dimensional structure and unique properties of unclassified proteins, which can ultimately lead to a diverse array of environmental, pharmaceutical and supplementary commercial applications. Distinctive proteins that are inadequately characterized or contain unfamiliar properties are cloned in the pMCSG19 vector and expressed in *Escherichia coli* BL21 (DE3) cells. Protein purification is essential in removing contaminants that have the potential to denature or modify the protein and leads to the production of high-quality, homogenous protein samples that can generate crystals. Accordingly, the cloned protein of interest is purified via two runs of immobilized metal ion affinity chromatography. This method is based upon the specific binding interaction between the amino acid histidine and the nickel ion. The specific protein is tagged with histidine and remains in the column bound to the immobilized metal ion. It is later eluted by the addition of a competitive molecule, such as imidazole, that displaces the His-tag from the nickel ion, and the tobacco etch virus protease is used to cleave the His-tag from the purified protein. The protein purification protocols are currently executed on AKTA XPRESS workstations capable of carrying out multidimensional chromatography. Synchrotron X-ray crystallography techniques at the Advanced Photon Source are used to determine the structure of the protein, and computational predictions of protein function are made and subsequently examined in enzymatic assays. All twelve of the proteins that underwent this process were effectively purified and all but four had the His-tag successfully cleaved. Those proteins that had sufficient protein yield were tested in two temperature conditions and are currently undergoing imaging to detect the formation of any crystals. Upon the formation of any crystals, X-ray diffraction will be conducted in an attempt to solve the protein structures. This information is highly crucial since the discovery of the structure and function of various proteins has the potential to augment the understanding of essential mechanisms of life and facilitate important advancements regarding health protection, medical developments, environmental renewal and energy production, among other applications.

Cloning, Purification and Crystallization of Mutant Adenovirus Proteinases

Jenny Wang (HARVARD UNIVERSITY, CAMBRIDGE, MA 02138), Walter Mangel (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Adenovirus proteinase (AVP) is a critical enzyme in the maturation of newly replicated adenovirus particles. The enzyme's importance in the viral life cycle makes it an attractive target for drugs to counter human adenovirus, a virus that has been implicated in respiratory illness and pink eye. To gain insight into the mechanism behind AVP activation and catalysis, we seek to identify key residues of the proteinase

and understand their role in AVP activity. Past studies on AVP have shown that the cysteine at the 122nd residue of AVP is the nucleophile needed for catalysis and substituting an alanine would prevent enzyme function. In addition, it is also known that a single mutation at the 137th residue of AVP from proline to leucine is sufficient to inhibit in vivo AVP activity at or above 39 °C and make virus particles non-infectious. With this information, we sought to express and purify these two mutant versions of AVP, one with cysteine mutated to alanine (C122A) and one with proline mutated to leucine (P137L) by cloning the mutated AVP gene sequence into a pET13a expression vector and introducing the vector into *Escherichia coli* cells. Although both C122A and P137L were successfully expressed by the *E. coli* cells, the P137L mutation rendered the recombinant protein insoluble and thus resistant to simple purification. Further tests suggested that urea at a concentration of 2 M may be needed to solubilize P137L. The readily soluble C122A protein was purified using cation-exchange and hydrophobic-interaction chromatography and crystallized in the presence of a synthetic peptide matching the sequence of a known AVP substrate. Using X-ray diffraction, we hope to solve the structure of this inactive C122A complex bound to synthetic peptide and use it to identify the interactions that bind active AVP to its substrates. This knowledge will open new avenues of targeted drug design against human adenovirus.

Metabolic Engineering of *Alicyclobacillus acidocaldarius* via Electroporation for the Production of Biodegradable Plastics

Mary Weston (DEPAUW UNIVERSITY, GREENCASTLE, IN 46135), Francisco Roberto (IDAHO NATIONAL LABORATORY, IDAHO FALLS, ID 83415). The gram-positive thermoacidophilic bacterium, *Alicyclobacillus acidocaldarius*, is being metabolically engineered to create a cost-effective and efficient bioprocess for the conversion of plant biomass into lactic acid, the precursor of polylactide, which is the main component of biodegradable plastics. Metabolic engineering is the alteration and optimization of genetic and regulatory processes in the cell. The bacterium is an excellent subject for engineering because it can function well in low pH, high temperature situations. In order to introduce new genetic information, tests were done with electroporation, where a brief pulse of electricity is applied to cells, causing the cell membrane to become permeable to foreign substances. Following electroporation, cells are able to reform the membrane with the foreign material remaining inside. In this project, electroporation was examined as an efficient strategy for inserting the plasmid pSUP104 into the bacterium. Plasmid DNA was added to rinsed cells and the solution was electroporated with a voltage between 1.4–2.5 kV and a resistance between 186–480 ohms. Multiple parameters and buffers were tested, but no bacterial transformants were observed. This could have been because the bacteria could not retain the plasmid or bacteria contained incompatible plasmids. Methodology changes to obtain transformants include growing bacteria in chemicals that weaken cell walls, using more voltage to increase membrane permeability, or using a different plasmid. After a plasmid is successfully transformed into the host cell then further gene manipulation can occur, such as enhancing the expression of certain genes and eliminating expression of others to promote the lactate dehydrogenase (LDH) gene. Additionally, the presence of the native LDH gene was verified for future purposes. *A. acidocaldarius* DNA was isolated and amplified via polymerase chain reaction (PCR). The product was sequenced, confirming the amplicon contained the native LDH gene. Lastly, a real-time PCR (Taqman) assay was designed to measure the expression of the LDH gene.

Tumor Necrosis Factor-α Increases Smooth Muscle Cell Proliferation

Sara Wezensky (UNIVERSITY OF LOUISVILLE, LOUISVILLE, KY 40059), Kara Kruse (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Angioplasty is a procedure that enlarges atherosclerotic vessel diameter via a balloon catheter, allowing for increased blood flow through the artery. Adverse consequences of balloon angioplasty, namely intimal hyperplasia (IH), occur in one-third of cases, and are not fully understood. Our team is currently developing a computation model of IH in order to elucidate mechanisms and pathways involved in the IH process. IH is characterized by the influx of cells from the media to the intima of an artery, causing restenosis. Major contributors to IH include activation of smooth muscle cell (SMC) phenotypic change, migration and proliferation. Migration is influenced by matrix metalloproteinases (MMPs), which degrade the matrix surrounding the SMCs, providing an avenue for motility. Immune contributions link the injury from the balloon catheter to the physiological changes in the vessel environment; immune cells and platelets providing the major thrust of chemotactic signaling after injury. Tumor necrosis factor-α (TNFα) is one chemical mediator released from endothelial cells, macrophages, mast cells and SMCs. We conducted an extensive literature search to determine the

degree that TNF α is chemotactic for SMC migration and involved in the induction of MMP activity. Specifically, we examined the biochemical pathways to identify the similarities between SMC migration and MMP activation, both induced by TNF α . By comparing the two pathways, we found that both use tumor necrosis factor receptor 1 (TNFR1), a 55-kD receptor. The 75-kD receptor, TNFR2, functions similarly to TNFR1, but is not activated in either pathway. Three adaptor proteins link both mechanisms as mediators in signal transduction: (1) TNFRSF1A-associated via death domain; (2) Fas-associated protein with death domain; and (3) TNF receptor-associated factor 2. SMC migration is activated through the nuclear factor-kappa B (NF- κ B) pathway, and MMP-9 activation occurs through the extracellular regulated kinase 1/2 mitogen-activated protein kinase (ERK 1/2 MAPK) pathway which then activates NF- κ B proteins. Thus, the initial and conclusive portions of both pathways are mediated through the same cell machinery. Our review provides a clearer look at mechanisms by which balloon injury may cause IH, and indicates that multiple mechanisms must be included in a computational model for it to accurately predict processes involved in intimal hyperplasia.

Quantifying Arbuscular Mycorrhizal Fungi Colonization Rates in Three Prairie Plant Species

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Although the symbioses between mycorrhizal fungi and many plant species are well documented, these symbioses are poorly understood. The prevalence of associations between plants and mycorrhizae makes understanding mycorrhizal fungi essential. Previous studies have shown colonization of mycorrhizal fungi is greater in plants with large unbranched taproots. For the current study, three prairie plants, wild quinine (*Parthenium integrifolium*), smooth blue aster (*Aster laevis*) and prairie dock (*Silphium terebinthinaceum*) were considered. Root samples were studied microscopically to determine colonization rates in the three species. Fungal in-growth bags were used to collect samples of extramatrical fungi, which were used in conjunction with the microscopically obtained colonization rates. The extramatrical fungi were also used in phospholipid fatty acid (PLFA) analyses. The PLFA analyses were performed on the fungi samples to determine the ratio of mycorrhizal versus saprophytic fungi. The prairie dock, which has a large unbranched taproot, was found to have the greatest amount of mycorrhizal colonization. The aster, which has fine highly branched roots, had the least colonization. The weights of the extramatrical fungi showed the same correlation. The PLFA analyses showed a greater presence of saprophytic fungi, which was expected because of the high nutritive value of prairie soils. These results add to the understanding of below ground traits of the study species. This information will be used to improve prairie conservation and restoration efforts.

Toward the Development of New Parkinson's Medicines: Production of the JNK3 T221E Active Mutant

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c-Jun N-terminal kinases (JNKs) are proteins expressed throughout the body. Isoform III (JNK3) is mainly expressed in the brain and has been directly linked to dopaminergic neuronal cell loss, a major symptom of Parkinson's disease. Therefore JNK3 is a good potential target for drug discovery. JNK3 is activated by the kinases MKK4 and MKK7 through phosphorylation of threonine 221 and tyrosine 223. JNK3 must be activated before substrate proteins can bind. This project aims to mimic active form of JNK3 by mutating threonine 221 to glutamic acid. Solving the crystal structure of this JNK3 T221E active mutant will provide a starting point for further drug discovery research. Using PCR the JNK3 T221E gene was amplified. The gene was cloned into the Invitrogen Gateway system and expressed in *Escherichia coli*. Once expressed, JNK3 T221E was purified using ion exchange chromatography. Sparse matrix crystallization screens were setup with the Art Robbins Phoenix robot using the purified JNK3 T221E. To date, diffraction quality crystals have yet to be obtained. This research represents the initial steps in a project to compare wild type JNK3 with the active mutant and to ultimately solve protein/substrate complex structures. These complexes will give researchers a better starting point for drug discovery efforts in the design of new medicines against Parkinson's disease.

G Proteins' Relation to Fungal Morphology of *Aspergillus niger*

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Heterotrimeric guanosine nucleotide-binding proteins (G proteins) are activated by signals from membrane associated G protein-coupled receptors (GPCRs). A GPCR receives a ligand or regulator on the extracellular surface and transmits the regulatory messages to the

G proteins, which ultimately leads to regulation of gene expression. This gene expression may affect the morphology of *Aspergillus niger*, which is critical for citric acid production. Understanding the way that gene transcription affects morphology could allow the use of fungi for high yield production of chemicals. In this study, three GPCRs (gprF, gprM and gprP) were studied via gene deletion. The double-joint PCR technique was used to build the gene deletion constructs, which contain the upstream region of the corresponding gene, an antibiotic marker gene (hygromycin) and the downstream region. The gene deletion constructs were prepared by PCR. These gene deletion constructs were confirmed by endonuclease restriction enzyme analysis. The constructs were separately introduced into *A. niger* by protoplast transformation and selected on minimal media with hygromycin. The hygromycin resistant mutants were grown for spore production. The spores were cultured in complete media for two days and then biomass was collected. Genomic DNA was prepared from the mutant biomass and used to confirm the gene deletion by PCR with a pair of primers, one of which was located within the selection marker gene and another outside the DNA sequence of the upstream (5') or downstream (3') regions. While all 29 samples (12gprF, 12gprM and 5gprP) showed some sign of proper insertion, only 5 out of 29 were found to have been inserted correctly in both the upstream and downstream regions without nonspecific fragments. The gene deletion will be further confirmed by Southern blotting analysis. After confirmation of the gene deletion, changes in morphology and citric acid production will be examined. This study will help define the GPCR's involvement in morphology and citric acid production in *A. niger*.

Towards the Generation of Human Embryonic Stem Cell Lines Expressing Oct4-Specific Green Fluorescent Protein

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Human embryonic stem cells (hESCs) are derived from the inner cell mass of preimplantation embryos; they can be cultured indefinitely and differentiated into different cell types in vitro. However, little is known about the factors that are important for maintaining undifferentiated hESCs in vitro. To investigate these factors, we aim to generate clonal cell lines that are able to express green fluorescent protein (GFP) reporter gene under the control of the Oct4 promoter. Since Oct4 is a critical marker of the undifferentiated state and a central regulator of pluripotency in hESCs, the generation of Oct4-specific GFP cell lines would provide a non-invasive method to monitor the expression of Oct4 and an invaluable tool to study the factors required for maintenance of undifferentiated hESCs in culture. Towards this goal, the promoter region of Oct4 was amplified from genomic DNA of hESCs by PCR which was subsequently digested by BamHI and XhoI, inserted into the promoterless vector, pAcGFP1-1 (Clontech), previously digested by the same pair of restriction enzymes, and transformed into competent cells of *Escherichia coli* DH5a. Plasmids were isolated from ten transformants and digested by BamHI and XhoI. At least one of the plasmids has so far been demonstrated to contain the insert which will be used to transfect hESCs once verified by sequencing.

* Crystallization Process of Protein Rv0731c from *Mycobacterium Tuberculosis* for a Successful Atomic Resolution Crystal Structure at 1.2 Å

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Proteins are bio-macromolecules consisting of 20 basic amino acids and have distinct three-dimensional folds. Determining the three-dimensional structure of a protein can help researchers discover the remarkable protein folding, binding site, conformation and etc, in order to understand protein interaction and aid possible drug design. Research focused on protein structure by X-ray protein crystallography is conducted by Li-Wei Hung's research group in the Physical Bioscience Division at Lawrence Berkeley National Laboratory (LBNL). The research in this lab is in the process of crystallizing the proteins to determine the three dimensional crystal structures of proteins. Most protein targets are selected from *Mycobacterium tuberculosis*. Tuberculosis (TB) is a possibly fatal infectious disease. Studying TB target protein can help discover antitubercular drugs and find a treatment for TB. The high-throughput mode of crystallization, crystal harvesting, crystal screening and data collection are applied to the research pipeline. The X-ray diffraction data by protein crystals can be processed and analyzed to result in a three dimensional representation of electron density, producing a detailed model of protein structure. Rv0731c is a conserved hypothetical protein with unknown function from *M. tuberculosis*. This paper is going to report the crystallization process and brief structure information of Rv0731.

Chemistry

Expression and Purification of Perdeuterated GFP for Neutron Diffraction Analysis

Rachel Applefield (EARLHAM COLLEGE, RICHMOND, IN 47374), Hugh M. O'Neill (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). The green fluorescent protein (GFP) isolated from the jellyfish *Aequorea victoria* has attracted great interest as a biological fluorescent marker and is one of the few examples of excited state proton transfer (ESPT) in nature. The GFP chromophore, a tripeptide comprised of the following amino acids: Ser65- Tyr66 - Gly67, must be in its anionic form to fluoresce. The anion is achieved through the deprotonation of the tyrosine residue. Neutron crystallography is noted for enabling the visualization of the positions of hydrogen atoms within a molecule. By using neutron crystallography, it may be possible to identify the hydrogen-bonded networks that stabilize the deprotonation of the chromophore leading to a more in-depth understanding of ESPT in GFP. In order to enhance the neutron diffraction data, crystals of perdeuterated GFP must be created. However, producing perdeuterated GFP is more difficult than expressing hydrogenated GFP. A vector containing the gene for the GFPmut3 from *A. victoria* under the tetracycline promoter was used to over-express GFP in *Escherichia coli*. Two growth media (Terrific broth and Enfors Minimal media) and two strains of *E. coli* (BL21 (DE3) and DH5a) were investigated in trial expressions of hydrogenated GFP in order to optimize the expression and purification process prior to over-expression in D₂O media. A unique system of purifying GFP was developed using three phase partitioning, anion exchange chromatography and gel filtration chromatography. This procedure yielded approximately 50mg GFP from a 200-ml culture. The purest fractions were then H/D exchanged using D-EPPS buffer. Crystallization trials are currently underway with the H/D exchanged GFP. *E. coli* BL21 that do not express GFP were identified during the trial expressions. It was noted that during the adaptation of *E. coli* BL21 to 100% D₂O media expression of GFP was lost because the non-expressing cells out-competed the expressing cells. Over-expression of perdeuterated GFP was achieved by limiting the number of passages and lowering the expression temperature to 30 °C. Subsequently, we have initiated the sub-cloning of GFP into the PET 11a vector to enable tighter control of GFP expression and eliminate the non-expressing population. To our knowledge, this is the first report of production of perdeuterated *A. victoria* GFP. In addition, observations made in this study will be broadly applicable to other protein deuteration studies.

Dependence of Physical Properties on Alkyl and Ether Chain Length with Phosphate Ionic Liquids

Steven Bagienski (RUTGERS UNIVERSITY, NEW BRUNSWICK, NJ 08901), James Wishart (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Ionic liquids are becoming more attractive to study due to their wide array of applications ranging from cellulose dissolution to storing gases. Ionic liquids are molten salts consisting of cations and anions, which tend to be viscous liquids below 100 °C. However, it is crucial to understand, as well as predict, the basic physical properties of these liquids before tailoring them for specific applications. This study concentrates on a series of phosphate ionic liquids consisting of N-butyl-N-methylpyrrolidinium phosphate (P₁₄PO₄), N-ethoxyethyl-N-methylpyrrolidinium phosphate (P₁EOEPO₄), 1-butyl-3-methylimidazolium phosphate (bmimPO₄) and 1-ethoxyethyl-3-methylimidazolium phosphate (EOEmimPO₄). Phosphate ionic liquids were chosen because the majority of the anions in existing ionic liquids are singly charged, while the phosphate anion is trivalent. The charge of the anion is a very crucial property in understanding why certain ionic liquids behave the way they do. The ionic liquids were prepared by mixing the corresponding bromide salts with N-methylpyrrolidine or 1-methylimidazole to create the bromine ionic liquid. Then the ionic liquids were metathesized to the phosphate ionic liquids using phosphoric acid. This series was characterized by measuring glass transition temperatures (T_g) with differential scanning calorimetry (DSC), decomposition temperatures (T_d) using thermal gravimetric analysis (TGA) and measuring their densities. The DSC scans showed onset T_g values of -53.7 °C, -71.69 °C and -66.43 °C for P₁EOEPO₄, EOEmimPO₄ and bmimPO₄ respectively. TGA scans indicated onset T_d values of 105.9 °C, 102.8 °C, 103.3 °C and 107.1 °C for P₁EOEPO₄, P₁₄PO₄, EOEmimPO₄ and bmimPO₄ respectively. Densities were measured to be 1.32 g/mL, 1.43 g/mL and 1.34 g/mL for P₁EOEPO₄, EOEmimPO₄ and bmimPO₄ respectively. The imidazolium cation ionic liquids were found to have a higher T_d than the pyrrolidinium analogs. The glass transition temperatures were lowest for the ether containing imidazolium ionic liquids. The highest densities were found to be the ether substituent imidazolium ionic liquids. While the densities mainly

depend on the molecular volumes, the correlation with the glass transition temperatures can be explained by the kinetic interactions between the cation and the phosphate anion. Further anticipated studies on the physical properties of ionic liquids include studying the effects of the charge on the anion in the ionic liquid by comparing phosphates to sulfate and nitrate ionic liquids as well as studies examining the liquids' polarities, viscosities, vibrational spectra and electrical conductivities.

Detecting Trace Ambient Pesticides in Real Time Using Single Particle Aerosol Mass Spectrometry (SPAMS)

Zachary Barker (MOUNT UNION COLLEGE, ALLIANCE, OH 44601), George R. Farquar (LAWRENCE LIVERMORE NATIONAL LABORATORY, LIVERMORE, CA 94550). Pesticides, by nature, are toxic substances, and may cause unintentional harm if improperly controlled. Given that pesticides are fairly ubiquitous, with wide use in agriculture and the household, and considering the potential for harm that pesticides pose to non-target organisms such as pets and humans, the detection of pesticides using rapid and effective means is particularly attractive. In this study, Single Particle Aerosol Mass Spectrometry (SPAMS) was used to demonstrate the rapid detection of five commonly used pesticides, often used in agricultural and home-and-garden applications. These include permethrin (pyrethroid class), malathion and dichlorvos (organophosphate class), imidacloprid (chloronitrotyl class) and carbaryl (carbamate class). Analytical standards of each compound were used to prepare a liquid solution through mixture with water or ethanol. The final liquid sample solution was aerosolized in a collision nebulizer to create particles for analysis in the SPAMS instrument. The resultant dual-polarity time-of-flight mass spectra were then analyzed to identify the characteristic peaks of the compound in the sample. In addition, samples of common household items containing pesticides, namely Raid™ Ant Killer 16 spray, containing permethrin, and a canine flea collar, containing carbaryl, were analyzed in their original state using SPAMS, without any further sample preparation. The characteristic peaks of the active pesticides in these samples were identified using the mass spectra obtained earlier from the pesticide analytical standards. By successfully identifying pesticides in analytical standards and in household items, it is demonstrated here that the SPAMS system is capable of pesticide detection in numerous agricultural and environmental situations.

Frequency Modulated Laser Absorption Spectroscopy of Singlet CH₂ in the Near Infrared Region

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The free radical methylene (CH₂) is an intermediate in many combustion reactions and has been subject of constant research for more than 40 years. In order to better understand CH₂, its rovibronic energy levels have been mapped out by spectroscopic analysis of the radical. To fill in some of the gaps in the experimental spectra, data were taken in the near infrared, a region that was notoriously hard to probe in the past. This new spectrum was combined with older spectra recorded by the Gas-Phase Molecular Dynamics group at Brookhaven National Lab for future analysis. CH₂ was synthesized through the photolysis of ketene by a 308-nm excimer laser. The spectrum was detected using a frequency modulated continuous wave diode laser in the range of 0.782 to 0.787 μm. The result of this project was the data itself. With this new data, new spectroscopic transitions can be assigned and derived energy levels can be reevaluated and compared to known data in the complete spectrum. The collection of this data is a small contribution to fully understanding the rovibronic energy structure of the methylene which will ultimately improve our chemical models of the combustion process.

Selective Electrochemical Oxidation of Sodium Chloride Solution

Max Bastow (COLORADO COLLEGE, COLORADO SPRINGS, CO 80903), Charlene Sanders (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Activated electrodes placed in saline solution create an electric double layer composed of opposite charges, repelling ions of like charge. It is hypothesized that, due to this characteristic of the electric double layer, it is possible to inject a short anionic pulse into a saline solution that will selectively oxidize water to produce oxygen. If the pulse is short enough, it will stop before chloride ions are drawn to the electrode surface, thus avoiding production of chlorine. This would have applications to the generation of oxygen and hydrogen from sodium chloride solutions. Phosphate buffered saline (PBS) was placed into an electrolysis cell and a stimulus generator was used for controlled charge injection of an anionic pulse. This pulse was applied for four hours in a closed cell and chlorine production was observed by the spectrophotometric determination of hypochlorite based on its reaction

with ascorbate. The same pulses were then applied to an identical cell containing PBS sparged with N_2 at 50 ml/min. A galvanic cell was used for oxygen measurements, and a Figaro gas sensor was used for hydrogen measurements. Evolution of chlorine was not observed until pulse widths greater than 200 μ s were applied. At this pulse width the production of oxygen was already well established at 0.11 ± 0.01 μ mol/hr. At the greatest applied pulse width of 400 μ s, chlorine production was at 0.053 ± 0.008 μ mol/hr while oxygen production was 0.25 ± 0.01 μ mol/hr. These results show that short pulses are indeed capable of oxidation of water in PBS to produce oxygen while avoiding the oxidation of chloride to chlorine.

Constructing Theoretical Three Dimensional Models of Glycosyltransferases Involved in Hemicellulose Synthesis Using Homology Modeling

Karole Blythe (LANGSTON UNIVERSITY, LANGSTON, OK 73050), Dr. Paul Adams (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). Plants are an inexpensive source of carbon, and therefore, are excellent candidates to generate an efficient biofuel. The process of producing biofuels from biomass requires the deconstruction of lignocellulose (cellulose, hemicellulose and lignin) into fermentable sugars. Unfortunately, hemicellulose binds tightly to cellulose and lignin forms a sturdy connection to the plant walls. Hemicellulose is also composed of high percentages of pentose monosaccharides, which are difficult to ferment. The complications of fermentation caused by hemicellulose are the main focus of this research. This study examines one method of better understanding hemicellulose, which is to create theoretical three dimensional models of the glycosyltransferases responsible for hemicellulose synthesis. The technique of homology modeling is used to construct the theoretical models. The names and amino acid sequences (query sequences) of genes encoding glycosyltransferases involved in hemicellulose synthesis were identified. MODELLER and BLAST programs were used to pinpoint protein sequences (templates) from the Protein Data Bank containing high similarities to the residues in the query sequences. Then, MODELLER was used for sequence alignments with each of the query sequences and templates previously identified. Finally, MODELLER calculated a theoretical model for each sequence alignment. The models chosen received the best MODELLER objective function score. Unfortunately, two of the models contain long strands of loops caused by the failure to align templates to certain regions.

Multiplexed Nanoparticle Assemblies for SERS Detection Applications

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In detection applications and microscopic analysis, Raman techniques offer advantages over well-established fluorescence techniques; however, low signal strength from Raman spectroscopy has limited its practical applications. To overcome these weak signal strengths, Surface Enhanced Raman Scattering (SERS), using metal nanoparticles as substrates for the attachment of the signal dye, has become increasingly utilized. To optimize the Raman signal, aggregation of silver (Ag) nanoparticles using salts enhances the Raman signal due to overlap of surface plasma resonance between the particles. Currently, alternative methods to control inter-particle distance using magnetic particles are also being researched. The strong signals from the Ag aggregates have allowed for combinations of different signal dyes for a single SERS-active nanoparticle. To achieve this, current research at Los Alamos National Laboratory involves synthesis of multiplexed nanoparticle assemblies to give a combination of signals. Ag nanoparticles approximately 60 nm in diameter were tagged with a particular Raman dye, aggregated and silica coated. The tagged Ag particles were attached to silicon microspheres via biotin-avidin interactions in different dye ratios. Raman spectroscopy and Raman microscopy were used to measure and characterize the signal strength of the particles. Results showed that the combination of different dye ratios on multiplexed nanoparticle assemblies maintained their fingerprint spectra, and the intensities of the individual peaks could be controlled by varying the concentration of added dye. Multiplexed nanoparticles can be used in further experiments requiring SERS-detection of different substrates simultaneously. Future synthesis of multiplex particles with different combination of dyes will allow for a larger array of dye spectra than currently available.

Imaging of Photosynthetic Solar Energy Flow in a Bacterial Membrane

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The conversion of solar energy to chemical energy through photosynthesis in the bacterium *R. sphaeroides* requires the absorption and dissipation of energy through a number of different membrane proteins. Understanding this process is crucial to the development of photosynthesis-inspired approaches to energy harvesting and conversion that use water as a main fuel source. The flow of solar energy can be observed between the individual cofactors in the reaction center (RC) by using transient spectroscopy, and on the membrane protein level through Atomic Force Microscopy (AFM) and Near-Field Scanning Optical Microscopy (NSOM). Measuring the absorption spectrum of the RC crystals and observing how the different components of the RC molecule absorb light at different orientations allows for the selective excitation of the different cofactors of the RC. Such selective excitation will be useful in further study of the mechanisms of solar energy transfer within the RC protein. In order to observe solar energy transfer among the many RC, light-harvesting 1 complexes (LH1), and light-harvesting 2 complexes (LH2) in the membrane on a multi-molecular level, AFM was used to obtain an image of the membrane proteins in a state where they are not exposed to light. Analysis of the effect of the directional orientation of light on absorption spectra has shown that it is possible to specifically excite cofactors in the RC. However, further mathematical work will have to be undertaken before such procedures become viable in the lab. AFM imaging of the *R. sphaeroides* membrane has revealed "train-track" patterns of pairs of dots, suspected to be membrane protein complexes, running across the membrane. However, no images clearly showed the arrangement of the individual light-harvesting complexes. Similarly, though PSI structures were observed, the AFM images did not reveal their organization in the membrane. Furthermore, further imaging using NSOM will have to be undertaken before a detailed image of the path of light transfer in photosynthetic membranes can be observed.

Development of Infrared and Raman Spectral Databases for Characterization of Hanford Tank Waste Samples

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Approximately 210 000 m³ of radioactive waste, generated as a result of past plutonium production processes, are being stored in tanks at the Hanford site in Richland, WA. Over the last 60 years some of these tanks have lost their structural integrity and have begun to leak harmful chemical and radioactive materials into the surrounding sediment and groundwater. The U.S. Department of Energy (DOE) and its contractors are developing means to treat and dispose of the radioactive Hanford tank waste. For the high-level waste (HLW), the solid fraction of the tank waste, the baseline pretreatment and immobilization strategy is to leach with aqueous sodium hydroxide (and with sodium permanganate for wastes high in chromium) and vitrify the leached solids in borosilicate glass. One of the main challenges to developing efficient pretreatment processes is the identification of the specific chemical species contained within the waste tanks. These waste tanks contain a complex mixture of inorganic compounds including various oxides/hydroxides of Al, Bi, Cr, Fe, U, etc. Inorganic mineral phases such as nitrate cancrinite ($Na_8[Al_6Si_6O_{24}](NO_3)_2 \cdot 4H_2O$) have also been observed in the soil around the tanks, formed by interaction of the tank material with surrounding sediment. In this study we have begun to construct a vibrational spectral database of potential waste components which will be used to spectroscopically characterize tank waste samples. Inorganic compounds were obtained from commercial sources with the exception of nitrate cancrinite, lanthanum(III) pyrophosphate, sodium uranium(VI) phosphate and iron(III) hydroxide which were synthesized according to published sources. The spectra of the various inorganic compounds were obtained using both Raman and Infrared (IR) spectroscopy. The spectra were entered into a database and labeled accordingly. The database was tested using spectra obtained from actual tank waste samples. The IR spectrum for one such tank waste sample was modeled using Microsoft Excel™ from the spectra of several inorganic compounds likely to be present in the sample. A reasonable fit to the experimental data was obtained, but the result indicated the actual tank waste material contained at least one unidentified component. Based on these results it can be concluded that IR spectroscopy and Raman spectroscopy hold potential as valuable tools for characterizing tank waste. These techniques may prove to be especially useful for amorphous solid compounds that cannot be identified by their X-ray or electron diffraction patterns.

Synthesis of Metal Acetylacetonates for Solid State NMR Studies of Paramagnetic Materials

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Nuclear Magnetic Resonance spectroscopy (NMR) has proven to be one of the most successful methods for learning about organic molecules in solution. Advances in NMR spectroscopy allow high resolution spectra to be obtained on solids, expanding the range of materials that can be studied by this technique. In this work diamagnetic and paramagnetic molecules are synthesized with the aim of using these substances to evaluate the use of solid state NMR as a characterization tool for paramagnetic solids. The solid state NMR work will focus on the ^{17}O isotope. The synthesis of a variety of metal acetylacetonate compounds, both paramagnetic samples and diamagnetic controls, labeled with NMR active ^{17}O , is reported. All have been evaluated using solution ^1H NMR for structure confirmation. The ^{17}O solid state spectrum of $\text{Al}(\text{acac})_3$ is similar to that of a carboxylate salt, revealing comparable electron delocalization in the acetylacetonate anion.

Dicyanoamide: Its Role in Energetic Ionic Liquids

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Energetic ionic liquids have drawn increasing interest as candidates for monopropellants with aerospace applications as their relative stability and high energy density surpass current fuels. The energetic ionic liquid 1,2,4-triazolium dicyanoamide [TZ^+/DCA^-] is investigated at the second order perturbation (MP2) level of quantum chemistry to determine the relative energies of the ion pair (TZ^+/DCA^-) and the neutral pair (TZ/HDCA), in which a proton has transferred from the cation to the anion. All of these calculations were completed using the 6-31++G(d,p) basis set implemented in the GAMESS software package. The ionization potential of DCA^- is determined using the equation-of-motion ionization potential coupled cluster (EOM-IP-CC) method in Qchem and the completely renormalized coupled cluster with single, double and triple excitations (CR-CC(2,3)) method in GAMESS, both with the aug-cc-pVTZ basis set. The proton transfer reaction: $\text{TZ}^+ + \text{DCA}^- \rightarrow \text{TZ} + \text{HDCA}$, is found to have net energy change of 4.212 eV. An approximation of the exact proton transfer energy is found using Hartree-Fock geometries for the ion pair and neutral pair. Single point MP2 energies for the two pairs give an energy difference of 0.4256 eV. The ionization potential is found to be 4.2486 eV using EOM-IP-CC and 4.123 eV using CR-CC(2,3). These results support TZ^+/DCA^- as an energy source that can be controlled by influencing the environment. Future studies include determining a catalyst to initiate the proton transfer reaction in the bulk of the ionic liquid.

* Polyaniline Nanofibers-Gold Nanoparticles Hybrids: Effects of Ring Substitution and Particle Sizes

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Polyaniline (PAni) is a conductive polymer that has some characteristics of a plastic and certain properties of a metal. One of its major properties is that it can be reversibly switched between a conductive or insulative form depending on the environment it is exposed to: acidic or basic. PAni nanofibers have been used in various sensor application because of their high surface area and their sensitive conductivity. Gold nanoparticles (Au-NPs) have also been used as sensors because of their nobility, resistance to surface oxidation and optical properties. This project combines PAni fibers or some of their analogs with Au-NPs of different sizes (11 nm–100 nm). In our studies, nanoparticles were prepared separately and then assembled to unite their unique characteristics and create a better nanomaterial. This project observed whether PAni and Au-NPs suffered any structural changes and how they attached to each other. The synthesis of PAni and other analogs requires a 4:1 ratio of aniline or other monomers and ammonium peroxodisulfate which acts as the oxidant. Each reactant is separately prepared in hydrochloric acid and then rapidly mixed at room temperature. To synthesize Au-NPs, a solution of gold chloride is boiled, then a solution of sodium citrate is added, followed by annealing. To characterize the new material, UV-Vis Spectroscopy, which was used to probe the electronic structure of PAni as well to identify the sizes of Au-NPs, showed size-dependent peaks from 520 nm to 600 nm. FTIR Spectroscopy was used to identify the chemical functional groups and the molecular structure of PAni and its chemisorption to Au-NPs. Scanning Electron Microscopy was used to observe the structure of the nanoparticles and showed that smaller Au-NPs attached better to PAni and other analogs than larger nanoparticles, and most importantly, the structures of the nanofibers and the nanoparticles were not disrupted. This work combines two different projects that aim to unite the special properties and functions of both PAni and Au-NPs to form a unique and novel hybrid nanomaterial that can be very useful for science and technology. It is also the beginning of a large project that aims to find

out the characteristics of this new nanomaterial and how it can be applied to invent better sensors and other similar materials.

Investigating Ionic Liquids for Biomass Fractionation

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Biomass is a complex material comprised mainly of cellulose. The highly crystalline structure of cellulose makes it insoluble in conventional solvents such as water and ethanol. Ionic liquids (ILs) are a new class of solvents which have received much attention recently. They have been deemed by many as "green" solvents because of their thermal stability, extremely low volatility and recyclability. In this study, two ionic liquids choline acetate (Ch Ac), and ethylmethylimidazolium acetate (EMIM Ac) were used for biomass fractionation. Both were easily recovered to be used again. Though the studies of these molten salts are far from complete, preliminary compositional analyses done by Microbac Laboratories, Inc. show that fractionation does occur, and ILs have definite potential to be used in future biomass processing for biofuels.

Models for Aging-Related Degradation of Structures and Passive Components in Nuclear Power Plants

Grant Cleavenger (ELIZABETH CITY STATE UNIVERSITY, ELIZABETH CITY, NC 27909), Jinsuo Nie (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

Brookhaven National Laboratory (BNL) recently entered into an agreement with the Korea Atomic Energy Research Institute (KAERI) to develop the technology needed to evaluate the degradation of structures and passive components (SPC) in nuclear power plants (NPPs), an important concern in determining whether or not to extend an initial NPP operating license from 40 to 60 years and in researching "life beyond 60" for NPPs. Improving technical information on aging-related degradation models for NPP SPCs will be beneficial in assessing the safety of NPPs. As one key research area in the BNL-KAERI collaboration, this study involves the identification of aging-related degradation models for the predominant materials used in NPP SPCs. Documents for license renewal applications and periodic safety reviews were surveyed and analyzed to select the predominant materials used in SPCs. Through this literature search, time-dependent models were identified for common degradation phenomena such as changes in material properties (e.g., strength, ductility, modulus), loss of material (e.g., corrosion, erosion) and cracking. The predominant materials used in the safety-related NPP SPCs have been found to be concrete, stainless steel, carbon steel and low-alloy steel. The identified and documented degradation models include six models for concrete, eight models for stainless steel and six models for carbon and low-alloy steel. These degradation models represent the state-of-the-art understanding of aging performances of the selected materials and will be used in the next phase of the BNL-KAERI collaboration which involves the time-dependent fragility assessment of NPP SPCs.

Identification of New Semiconductors: Synthesis and Band Gap Measurements Using Reflectivity

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The search for new radiation detectors at Lawrence Berkeley National Laboratory has been carried out by high throughput synthesis and characterization of inorganic compounds. Semiconductors like high purity germanium (HPGe) currently serve as efficient gamma-ray detectors, but only at low temperatures. Discovery of high-quality semiconductors that are operational at room temperature can be arduous and lengthy. New characterization methods are needed in order to quickly analyze semiconductor candidates. By measuring band gaps using high throughput diffuse reflectivity measurements, new candidates for semiconductor gamma-ray detection can be easily identified. Dark compounds were chosen for analysis with the assumption that their band gaps will be in the targeted range of 1.2 to 2.5 eV. Other compounds with an estimated band gap in that range were also synthesized. The identities of the powdered samples were confirmed by X-ray diffraction, and diffuse reflectivity measurements were completed for each sample. Of the 63 compounds considered, HgI_2 , PbI_2 , CdS , BiPbO_2I , BaLa_2S_4 , LaVO_4 , BiOI and Pb_5O_{42} had band gaps within the desired range and should be further explored as semiconductors. It was determined that substituting a heavier element in some cases can lower the band gap of a compound.

Techniques to Increase DESI-MS Signal Intensity of Proteins

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Desorption electrospray ionization-mass spectrometry (DESI-MS) is an open air surface sampling/ionization technique that combines easy sample preparation with a capability for high throughput analysis. Our

group is investigating the desorption/ionization process with the goal of elucidating ways to substantially increase desorption/ionization efficiency, and thus, increase overall analyte signal intensity in the mass spectrum. In this study, we examined the effectiveness of various techniques for increasing DESI-MS signal of analytes deposited or separated on thin-layer chromatography (TLC) plates. The signal level of selected compounds desorbed/ionized from these plates was examined with acidic or basic modifiers added to the DESI spray solvent and TLC plate, following derivatization of the analytes on the plate, heating the plate and heating the atmospheric sampling capillary. The spray solvent was modified using 0.1% formic acid and 0.1% ammonium hydroxide. Peptide derivatizations were attempted using the common protein stains fluoescamine, ninhydrin and O-phthalaldehyde. Acidic and basic modifiers proved ineffective in increasing overall intensity except in one case, and derivatization with protein stains only further complicated the spectra. Heating of TLC plates led to a variety of results for peptides tested. An increase in signal was observed for leucine enkephalin (YGGFL), and acetyl-RAYFAVR, while the bradykinin spectra revealed more fragmentation. A series of dipeptides was tested with varying solvents at different plate temperatures, which showed more fragmentation with increasing temperature. We also examined the effects of heating the atmospheric sampling capillary. For YGGFL and bradykinin, a total increase in signal was observed upon heating. More importantly, an increase in the $[M+H]^+$ and $[M+2H]^{2+}$ species were seen for each peptide respectively. Of all the methods investigated, heating the atmospheric sampling capillary provided the most benefit in terms of analyte signal enhancement.

*** Computational Investigation of the Effect of Oxidation State on Conformational Ensembles: Applications to Possible Molecular Wires for Solar Energy Devices**

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Abstract Biological systems rely on heme-proteins to carry out a number of basic functions essential for survival. One class of heme-proteins, C-type cytochromes, found in a variety of bacteria, plants and animals, were studied as possible building blocks for solar energy devices because of their ability to initiate electron transfer (ET). The C7 protein was chosen because (1) experimental scattering data are available and (2) it has three heme sites, making the effect of oxidizing or reducing the iron in the center of the site larger than for proteins with single hemes. To assess their suitability for ET devices, their solution conformations must be determined. Experimental solution-phase X-ray scattering studies have found that the C7 type cytochrome, extracted from the *Geobacter* genome and expressed in *Escherichia coli*, has identifiably different solution-state conformations in the reduced and oxidized form. The current work seeks to determine what conformational changes produce the experimentally observed differences in the scattering spectra. A starting structure obtained from crystal structural data (Protein Data Bank entry 1os6) was subjected to nanosecond scale constant pressure and temperature molecular dynamics simulations in a 50x50x50 Angstrom cube of water using the Chemistry of Harvard Molecular Modeling (CHARMM) program. The calculations reproduced the observed scattering differences between the oxidized and reduced states. The role of several lysine residues and the n-terminus group in the electrostatically driven conformational change upon oxidation were investigated. These results demonstrate that molecular dynamics (MD) combined with X-ray scattering is an effective way to assess ensemble conformations.

Temperature Dependence in the Reduction Kinetics of Fe(III) Complexes by Cytochromes STC and Soluble and Membrane OmcA of *Shewanella oneidensis* MR-1

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Dissimilatory metal reduction by bacteria (DMRB) has profound consequence in the reductive dissolution of the metal oxide solids and mineral phase transformation. In environmental science, DMRB can be potentially employed in bioremediation of toxic heavy metals as well as high oxidation state radionuclides such as uranium and technetium in soils and sediments. Certain cytochromes of *Shewanella oneidensis* MR-1, such as MtrC, OmcA and the small tetra-heme cytochrome (STC), play key roles in the reduction of both soluble and insoluble metals and metal complexes. The reduction of Fe-ligand complexes by heme-based cytochromes offers an ideal system for understanding the microbial reduction of metal ions. Further insight into this reduction process can be gained through a systematic study of this electron transfer process over a range of temperatures. In this

project, the reduction kinetics of ferric complexes with citrate, NTA and EDTA by three cytochromes from MR-1 including membrane OmcA, soluble OmcA and STC are studied by stopped-flow technique in the temperature range from 10 °C to 55 °C. The objective of this work was to investigate the effect of temperature on the reduction kinetics and delineate the relationships between the kinetic properties and the complexes and proteins as they pertain to this process. Stopped flow measurements were performed using a temperature controlled SFM-400 stopped flow system in junction with an MOS-250 spectrometer enclosed in a nitrogen filled environmental chamber. Microliter amounts of reduced protein and Fe(III)-ligand complexes were mixed rapidly and injected into a cuvette. The reduction of the Fe(III)-ligand complexes was indirectly monitored by way of observing the oxidation status of the protein indicated by the diminishment of an absorbance peak at the 552 nm wavelength. The redox reaction proceeds over a range of temperatures (10–55 °C). The reactions complete in less than an hour. The reaction rate generally increases as the temperature increases except at temperature >45 °C, after which the reaction sharply slows down, suggesting possible denaturation of the proteins. The kinetics curves were modeled by pseudo first order (exponential) decay curves. Generally at all temperatures the decay (reaction) rates increased in the order of: Fe(III)-Citrate<Fe(III)-NTA<Fe(III)-EDTA for Soluble OmcA and STC; STC<Membrane OmcA<Soluble OmcA for Fe-citrate; STC<Soluble OmcA for Fe-NTA and Fe-EDTA.

In Situ Studies of CeOx/CuOy Catalyst during the Water-Gas Shift Reaction using X-Ray Diffraction and X-Ray Absorption Near-edge Spectroscopy

Michael Estrella (St. FRANCIS COLLEGE, BROOKLYN, NY 11201), Jose Rodriguez (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Hydrogen is a potential alternative energy source to help us meet our ever-increasing energy needs. In this work, we studied the H₂ production from the water-gas shift (WGS) reaction over CeOx/CuOy catalysts. The WGS reaction is used for hydrogen production in fuel cell systems. In fuel cell systems, CO concentrations must be less than 10–20ppm in the presence of about 35% H₂ to avoid poisoning the Pt electrode. Currently, there are industrial catalysts such as Fe/Cr and Cu/Zn/Al that decrease CO poisoning via the WGS reaction. Yet these catalysts require lengthy and complicated activation steps before usage. Thus, we seek to develop a more versatile catalyst, and it is this impetus that drives our research. Our goal is to garner a fundamental understanding of the structure and properties of our catalyst at its active sites during the WGS reaction so that we can enhance the rational design of future catalysts for better efficiency. In situ X-ray diffraction (XRD) experiments were carried out on beam line X7B and in situ X-ray absorption near-edge spectroscopy (XANES) experiments were carried out on beam line X19A of the National Synchrotron Light Source at Brookhaven National Laboratory. We used the XRD powder patterns and XANES data to characterize our catalyst and monitored the catalytic performance using mass spectrometry (MS). In our set-up, we had in situ production of H₂ carried out in a flow cell with a 5% CO gas stream bubbled through H₂O. Our XRD analysis revealed that our catalyst was reduced from the copper oxide phase to the metallic copper phase during the WGS reaction. This occurrence coincided with an increased production of H₂ and CO₂. Our XANES data corroborated our XRD data, with yet more precision because we were able to observe the in situ runs at both the Copper K-edge and the Ceria LIII-edge. We were also able to readily oxidize and reduce our catalyst without compromising its performance. Thus, we were able to correlate the structural transformations with catalytic activity by demonstrating that metallic copper is the active phase for H₂ production. Partial reduction of ceria was also observed in the XANES data and was attributed to oxygen vacancies. These vacancies are also correlated with increasing catalytic activity. This work is part of a continuing study to understand the active sites for the WGS reaction on CeOx/CuOy catalysts and demonstrates the advantage of in situ studies for heterogeneous catalytic reactions.

Alternate Separations Scheme for Radiochemical Analyses of Fission and Activation Products in Irradiated Nuclear Materials

John Fain (UNIVERSITY OF CALIFORNIA—DAVIS, DAVIS, CA 95616), Matthew Douglas (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352). For applications in waste remediation and national security, methods for the analysis of mixed fission products from irradiated nuclear materials are being further developed. Due to the complex nature of irradiated samples, efficient separations are necessary for proper quantification of target analytes. As an alternative to existing separation schemes, portions of a newly-proposed method were investigated utilizing inductively-coupled plasma optical emission spectroscopy (ICP-OES) for quantification. A neat elemental standard containing 21 elements

was prepared, subjected to calcium fluoride (CaF₂) precipitation and the precipitate dissolved to undergo ion-exchange chromatography according to the proposed scheme using commercially-available columns. Both the initial supernate and the fractionated precipitate eluates were analyzed via ICP-OES. Initially, most elements thought to precipitate with concentrated HF did so, with the exception of cadmium, which showed no significant precipitation. Others, such as beryllium and barium, partially precipitated. Analysis of ion exchange chromatography fractions showed that many elements eluted at the hypothesized stage of separation, notably beryllium with nearly a full recovery during its elution. Others, such as strontium, were not found in significant concentrations at their predicted point of elution. Although some elements were not isolated predictably, or at all, many were found to elute at least partially under the conditions in the proposed scheme. This indicates that the proposed method may be largely effective but requires refinements in the conditions for ion exchange chromatography to improve the degree and efficiency of separation.

The Impact of Electrolyte Degradation on Lithium Ion Battery Performance

Daniel Fink (UNIVERSITY OF ROCHESTER, ROCHESTER, NY 14627), **John B. Kerr** (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). This study explores the effects of heat and water contamination in the electrolyte solutions containing LiPF₆ salts commonly used in lithium ion batteries. Evidence is presented that verifies the occurrence of unwanted side reactions which degrade the performance of the battery. The behavior of LiTFSI based electrolyte was also examined as a control. The equilibration of LiPF₆ to form PF₅ (g) in situ results in ring opening of the electrolyte component, ethylene carbonate (EC), and its reaction with H₂O to form HF and PF₃-O, strong Lewis acids. Several solutions with different water contents were prepared and placed under heat (50 °C) with intermittent analysis to determine variations in water content, viscosity, composition, anion presence and oligomer/polymer formation. Electrolyte solutions prepared with LiPF₆ exhibited a 10–15% increase in viscosity over a one week period under heat in part due to the high rate of formation of transesterification products as well as the production of ethylene oxide based oligomers observed in the GC analyses. Also detected was the formation of large PEO-like polymers and their further reaction products with the Lewis acids, PF₅, PF₃-O and HF. Analysis with HPCE exhibited peaks of the phosphate anion that increased with time under heat revealing further evidence of the breakdown of LiPF₆ and its reaction with the ethers in solution. Cells (anode/Li) were assembled with the electrolyte solutions at different stages of the analysis and cycled. Impedance spectroscopy followed each lithium insertion and extraction. This analysis displayed increased interfacial impedance with pre-heated electrolyte solutions as compared to those stored at room temperature possibly due to the presence of high molecular weight polymers on the electrodes. These results coupled with previous studies indicate that LiPF₆ is unstable in the carbonate solvents commonly used to prepare electrolytes for lithium ion batteries and needs to be replaced.

Absolute Energy Finding Application for CH₂ in Java

Eric Friedlander (RICE UNIVERSITY, HOUSTON, TX 77005), **Trevor Sears** (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Radical methylene is a common reaction intermediate in many combustion reactions. More extensive knowledge of its behavior could lead to cleaner and more efficient reactions. We can study this molecule using spectroscopy. When a molecule is excited to an elevated state, it can only be excited from one of several lower states given by a set of selection rules that are specific to the given molecule. These selection rules arise from quantum mechanics and the fact that almost every aspect of a molecule (spin, shape, etc.) is quantized. When the spectrum of the molecule is taken, the differences in energy of the set of lower energy levels that transition to a given excited states will correspond to the differences in energy between peaks on the spectrum. Therefore, the proper peaks can be located using these differences. Once the peaks for a given excited state are located, the absolute energy of the excited state can be calculated by adding the energy of the lower state with the transition energy given by the wavelength of the peak on the spectrum. Using Java, a program was implemented that uses these selection rules to calculate the set of lower energy levels and from them the energy difference, and then scans the spectrum for these differences. Once it finds the set of the peaks that lead to the excited energy state, it calculates that state's energy by adding the lower energies to the transition energies given by the peaks. Once the spectrum for CH₂ is available, it will be possible to calculate the energies of the excited energies. The spectrum of CH₂ is extremely extensive and takes months to fully assemble. As a result, the full spectrum of the molecule was not fully analyzed and

the program remained unused. Once the spectrum becomes available and the spectrum is assessed, the information will, hopefully, lead to more knowledge dealing with the behavior of radical intermediates in combustion-like reactions. Once the behavior of CH₂ is analyzed, the knowledge can be applied to combustion-like reactions in which CH₂ is an intermediate. Many of these reactions are pertinent to organic reactions used for power. As such, the knowledge of CH₂ would be useful in creating cleaner and more efficient reaction pathways in these reactions.

Thickness Determination of Diamond Stripper Foils for the Spallation Neutron Source

Dan Gardner (ILLINOIS STATE UNIVERSITY, NORMAL, IL 61761), **Robert W. Shaw** (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). To obtain high energy protons in proton accelerators, physicists first accelerate hydride ions and pass these ions through a carbon-based stripper foil. The foil strips electrons from the ions, leaving high-energy protons. This method of proton production is used at the Spallation Neutron Source (SNS). The high-energy protons are aimed at a mercury target, which spalls (ejects) neutrons. The SNS power is scheduled to increase so our group has previously done work to grow stronger stripper foils to handle the increased power. Here our research focused on determining the thickness of these foils in a non-destructive way. It is highly desirable to know the thickness of the foils, as foil thickness greatly affects both the stripping efficiency and the beam scattering. Unfortunately, all methods used thus far to determine foil thickness destroy the tested foil. Average thickness calculated from the foil mass, width and length has been reported in the past, but this average may not be representative of the thickness at the spot through which the beam passes. Here we have used alpha spectrometry to measure foil thickness at the location through which the SNS beam passes, without damaging the foil. Samples of americium-241 were used as a source of alpha particles; these particles lose energy as they pass through a foil. For calibration purposes, the foils were then broken to allow us to make thickness measurements with scanning electron microscopy (SEM). The SEM measurements were then used to relate the alpha energy losses to the physical thickness. The geometry of the apparatus was arranged such that the alpha particles pass through the same area of foil as the SNS proton beam. Our results show that the alpha spectrometry experiments can determine foil thickness within +16 nm. The overall accuracy of the experiment is limited mainly by the energy resolution of the alpha-particle detector. Future foils delivered to the SNS will use this technique to report foil thickness, rather than depending on the previous convention of reporting a foil's average thickness.

Analytical Method for the Identification and Quantification of Pinitol in Plant Roots by Gas Chromatography/Mass Spectrometry

Shaun Garland (UNIVERSITY OF CALIFORNIA—DAVIS, DAVIS, CA 95616), **Steven Goheen** (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352). Pinitol (D-3-O-methyl-chiro-inositol), a cyclitol, is thought to have a variety of roles in plant biology. However, new applications of pinitol for potential medical use are currently being investigated, increasing the importance of finding and determining the pinitol content in plant sources. While plant tissue extraction and trimethylsilyl imidazole (TMSI) derivatization methods for the analysis pinitol are typically discussed in literature, the extraction and analytical processes together with the mass spectra have not been reported in detail. In this work a reliable method for the identification and quantification of pinitol using TMSI derivatization and gas chromatography/mass spectrometry (GC/MS) is presented. Roots from soybean plants (Glycine max) were homogenized in methanol, filtered, dried and reconstituted in a known volume of methanol. Aliquots of the extract were then dried, derivatized with TMSI, diluted with toluene and analyzed by GC/MS. The chromatogram and mass spectrum of TMSI-derivatized pinitol are shown and discussed. Pinitol concentrations of 1930 ± 290 µg/g fresh weight (FW) were found in the soybean roots. A method to identify pinitol using its major ion fragments is given. An accurate mass measurement of the major ion fragment observed at m/z 260 was performed to determine its chemical composition. As the importance and utility of pinitol becomes better established in pharmacology and plant physiology, analytical methods such as the one described here will become increasingly valuable tools for identifying and quantifying pinitol concentrations in various phytochemical sources.

Removal of Actinides from Fuel Samples Using Manual Gas Pressurized Extraction Chromatography with TRUTM Resin Column

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Advanced fuel samples containing plutonium, americium and uranium need to be characterized to identify any trace impurities before insertion into a reactor. The characterization of the fabricated fuels is accomplished by using inductively coupled plasma mass spectrometry (ICP-MS) with gas pressurized extraction chromatography (GPEC). The chromatography system removes the actinides from the matrix, which allows for simpler analyses, less exposure to personnel and lower detection limits for the analytes of interest. TRUTM resin column was tested for ability to remove actinides from surrogate samples in both nitric acid and hydrochloric acid matrices; which are commonly used to dissolve the samples. Next, verification of the compatibility of the TRUTM resin column with trace elements was determined on the ICP-MS. Lastly, the method developed was applied to real fabricated fuel samples containing 80% plutonium and 20% americium. The TRUTM resin with nitric acid matrix worked well for the retention of plutonium and americium. Trace elements in nitric acid matrix were able to pass through the TRUTM resin column unretained with the exceptions of lanthanides, yttrium, zirconium and molybdenum which either partial or fully retained on the column. TRUTM resin with hydrochloric acid matrix worked well for the retention of uranium and plutonium but was unable to retain americium due to a low k' value. Hydrochloric acid matrix looks promising for trace metal determinations. However, contamination of concomitant elements in the load fraction made quantification in low ppb levels difficult. Further investigation into the source of the contamination is needed. The method was applied to real fuel samples in a nitric acid matrix. The results were extremely promising. There was no plutonium or americium in the load fraction and recoveries were nearly 100%. Modification of the strip solutions or number of strips should increase recoveries.

The Synthesis and Characterization of New, Robust Titanium (IV) Scorpionate Complexes

Jared Gerschler (HAMPSHIRE COLLEGE, AMHERST, MA 01002), James F. Dunne (IOWA STATE UNIVERSITY, AMES, IA 50011), Aaron Sadow (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352). Titanium complexes possessing sterically encumbered ligands have allowed for the preparation of reactive moieties (imido, alkylidene and alkylidyne species) relevant to reactions such as olefin polymerization and alkene hydroamination. For this reason, we have targeted robust scorpionate ancillary ligands to support reactive titanium centers. Thus, a series of titanium complexes were synthesized using an achiral oxazoline-based scorpionate ligand, tris(4,4-dimethyl-2-oxazolynyl)phenyl borate $[To^M]$ as well as the related chiral ligand, tris(4-isopropyl-2-oxazolynyl)phenyl borate $[To^*]$. The complex $[Ti(\kappa^3-To^M)Cl_3]$ was prepared in moderate yield (43%) by the rapid (<1 min at room temperature) reaction of $Li[To^M]$ and $TiCl_4$ in methylene chloride; this new compound was characterized by ^1H NMR spectroscopy as the expected C_{3v} -symmetric species. One route to Ti (IV) alkyls involves salt metathesis; accordingly, syntheses of $[To^M]Ti$ alkyl complexes by interaction of $[Ti(\kappa^3-To^M)Cl_3]$ and one or three equivalents of alkylating agents, such as benzyl potassium ($KCH_2C_6H_5$), trimethylsilylmethyl lithium ($LiCH_2Si(CH_3)_3$), or neopentyl lithium ($LiCH_2C(CH_3)_3$) are currently under investigation. The complexes $[Ti(=NBu^t)(\kappa^3-To^M)(Cl)(Bu^tpy)]$ ($Bu^tpy=4$ -tert-butylpyridine) and $[Ti(=NBu^t)(\kappa^3-To^P)(Cl)(Bu^tpy)]$ were synthesized by reaction of the known Ti imido $[Ti(=NBu^t)(Cl)_2(Bu^tpy)_2]$ with $Li[To^M]$ or $Li[To^*]$, respectively, by stirring overnight in methylene chloride at ambient temperature. The complexes were identified using ^1H NMR spectroscopy, ^1H - ^{13}C HMQC and ^1H - ^{15}N HMBC correlation experiments.

Chemical Sensor for Detection of Organophosphorus Pesticides in Water

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Ensuring the safety of the Nation's food and water supply is a critical national priority. The objective of this study was to develop and test a chemical sensor to detect organophosphorus pesticides in food or water; these pesticides may be present as a result of inadvertent or deliberate contamination. The benefits of sensor technology for such applications are: portability, ease of preparation, low cost, reliability and ease of operation in comparison to standard analytical techniques (i.e., gas chromatography — mass spectrometry, or high-performance liquid chromatography). Sensor coating materials sensitive to analytes of interest were developed and tested on quartz crystal microbalance (QCM) transduction platforms. The molecular imprinting technique was used to develop these coating materials. Scanning electron microscopy (SEM) was utilized to characterize films made from the molecularly imprinted polymer (MIP) materials. The SEM micrograph showed that the film was a composite nanostructured material with

the smallest particles measuring approximately 50 nm in diameter. The MIP materials were interfaced with mass-sensitive QCM sensor transducers, and the resulting sensors were tested for their ability to detect selected pesticides in water. The sensors showed a decrease in operating frequency and an increase in resistance upon being exposed to trace levels of the pesticides. When exposed to pure water, the sensor regenerated, demonstrating a reversible response (retuning to the baseline response when exposed to water). Future studies will attempt to optimize the imprinted nanomaterials to make the sensors more robust and more selective.

Finding Optimal Ion-Solvent Configurations Using FTIR Spectroscopy for Studying Ion Association and Dissociation Dynamics in Thiocyanate Salt Solutions by 2DIR Spectroscopy

Maria Gonzalez (LOYOLA UNIVERSITY, NEW ORLEANS, LA 70118), Kelly Gaffney (SLAC NATIONAL ACCELERATOR LABORATORY, STANFORD, CA 94025). Understanding the ultrafast structural dynamics of complex molecular systems in solution has been restricted by the fast time scale of such processes, limiting the understanding of very basic chemical processes. Recently, two dimensional infrared spectroscopy (2D-IR) has been used to probe molecular dynamics under thermal equilibrium conditions occurring on femto- and picosecond time scales. The ion association and dissociation dynamics in thiocyanate salt solutions will be probed using 2D-IR spectroscopy allowing for the determination of equilibrium association (or dissociation) rate constants of the thiocyanate anion and its counter cation as well as their dependence on the interactions with surrounding solvents. Vibrational modes of thiocyanate ion (NCS⁻), which were sensitive to ionic configurations (free ion and contact ion pair forms), were used as probes in studying the association and dissociation equilibrium dynamics between the thiocyanate ion and its counter cation in solution. The ion-solvent configurations in the thiocyanate salt solutions optimal for 2D-IR spectroscopy were determined by a one to one area ratio of the NCS⁻ peaks in free ion and contact ion pair forms using Fourier transform infrared (FTIR) spectroscopy. Optimal ion-solvent configurations for lithium thiocyanate, sodium thiocyanate and potassium thiocyanate were respectively determined to be 0.040 ± 0.002 M lithium thiocyanate in diethyl ether with $0.118 \text{ mols} \pm 0.001$ of lithium chloride, 0.060 ± 0.003 M sodium thiocyanate in acetonitrile and 0.050 ± 0.004 M of potassium thiocyanate in methanol.

Effect of Atomic Layer Deposition Support Thickness on Structural Properties and the Oxidative Dehydrogenation of Propane on Alumina and Titania-Supported Vanadia

James D. Dreessen, Anne M. Grady, Grigoriy Sereda and Mark Turner (UNIVERSITY OF SOUTH DAKOTA, VERMILION, SD 57428), Joe Libera and Christopher Marshall (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). Considering that the global demand of propylene is expected to rise above that of production, it is important to find novel, efficient ways to produce propylene in an industrial setting. Vanadium catalysts have shown possibilities of increasing the efficiency and production of propylene. The catalytic and structural properties of Al_2O_3 , TiO_2 and SiO_2/Al_2O_3 supported vanadia have been examined for the oxidative dehydrogenation (ODH) of propane. The purpose of the structural and catalytic testing is to elucidate when the support will behave as a separate phase rather than a cross between the new support and the base silica and to evaluate the performance of each catalyst. Atomic layer deposition was employed to create thin films of Al_2O_3 and TiO_2 on silica that range from a thickness of one to twenty alumina or titania units (cycles). These engineered solid supports were then loaded with vanadia via incipient wetness impregnation. Catalytic properties (selectivity, reactivity and the apparent activation energy of propane ODH) were determined from kinetic measurements performed with a flow reactor and an inline-gas chromatograph. Powder X-ray diffraction (XRD) was used to provide detailed information about the chemical composition and crystallographic structure of the catalyst. Electronic properties were studied by UV-Vis spectroscopy. The reducibility of the catalysts was analyzed using temperature programmed reduction with H_2 . Morphology of the prepared catalysts (surface area, pore volume, diameter and distribution) was studied by nitrogen adsorption (BET-equation and BJH-plots). Analysis of methods showed that ALD catalysts did not act like the silica starting material or the bulk control material.

Synthesis and Toxicity of Pyrrolidinium Ionic Liquids

Jinhee Gwon (QUEENSBOROUGH COMMUNITY COLLEGE, BAYSIDE, NY 11365), Dr. James Wishart (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Attention given to the field of ionic liquids (ILs) has been increasing lately because of their potential uses as green solvent alternatives due to their relative non-volatility, non-flammability, high conductivity and also wide liquid range compared to volatile organic solvents. But it is

critical to know and understand their toxic effect on the environment before actually replacing the current solvents with them. There have been a few reports suggesting that ILs are toxic to organisms varying from nematodes to algae and fish; however, there have not been many studies, if any at all, that have showed the relationship between the purity based on the color of the ILs and their toxic effects. Therefore, a series of halide salts based on N-methylpyrrolidine was successfully prepared in different levels of purities. N-methylpyrrolidine was reacted with alkyl halides of various chain lengths to produce the corresponding quaternary ammonium halide salts. These alkyl halides include 1-Bromobutane, 1-Bromopentane, 1-Bromodecane, 1-Bromododecane and 1-Bromooctadecane. The different levels of purities were achieved by using a different amount of heat to the reactions. The resulting quaternary ammonium halide salts were purified by washing with ethyl acetate and diethyl ether. The structures of the salts were confirmed using ^1H and ^{13}C Nuclear Magnetic Resonance (NMR) spectroscopy. The next step consisted of converting the salts to ionic liquids bearing the phosphate (PO_4^{3-}) and bis(trifluoromethylsulfonyl)imide (NTf_2^-) anions. These liquids were prepared with different levels of purities and in addition to NMR, UV Visible absorbance spectroscopy was used to test the ILs' purity. Then these ILs were screened for their toxicity to a variety of organisms including mold (*Rhizopus stolonifer*), plant (*Arabidopsis thaliana*) and insect (*Anopheles stephensi*). This is a part of a larger collaborative research project where other similar series of ionic liquids will be prepared and the liquids will then be screened for their toxicity to a variety of organisms.

Lipid Production by *Nannochloropsis oculata* in Batch Culture: The Role of Nitrogen Limitation

Blake Herron (WASHINGTON STATE UNIVERSITY—PULLMAN, PULLMAN, WA 99163), Michael Huesemann (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352).

With the advent of higher oil prices and the threat of climate change, the demand for alternative energy sources has never been higher. Specifically, biofuels have received a great deal of attention. Currently, biofuel production primarily utilizes terrestrial crops as a feedstock (e.g., corn and soybean for ethanol and biodiesel, respectively). This, however, has resulted in increased food prices and food shortages since there is not enough fertile land to provide both food and biofuel. The production of biodiesel from microalgae lipids is a promising alternative to terrestrial plants. Microalgae are far more productive, do not require land used for conventional agriculture, utilize wastewater and produce valuable co-products. This study focuses on the synthesis of lipids by *Nannochloropsis oculata* under nitrogen limitation, to be used as a possible feedstock for biodiesel production. *N. oculata* was grown in four culture bottles at 0.5, 1.0, 1.5 and 2.0 mM nitrate at a light intensity of 100 $\mu\text{moles}/\text{m}^2\text{s}$. Once nitrogen has been consumed, the nitrogen-deficient medium causes rapid lipid synthesis and accumulation. The cellular lipid content of *N. oculata* under these nitrogen deficient conditions reached maximums of 22 to 31%. When the medium became nitrogen-deficient, lipid concentration in culture peaked at 155 mg/L while lipid productivity reached 27 mg/L $\cdot$ day. While several *N. oculata* strains reported in the literature exhibit high lipid productivities and thus may have potential as a feedstock for biodiesel production, this strain demonstrates relatively low cellular lipid content, low lipid productivity and a low maximum culture lipid concentration at a light intensity 100 $\mu\text{moles}/\text{m}^2\text{s}$, making it a less suitable feedstock in comparison to other highly productive species.

Development of an Organocatalytic Method for the Direct Incorporation of $^{11}\text{CO}_2$ in Pharmaceuticals

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Positron emission tomography (PET) is a technique that has allowed researchers to study pharmacokinetics and pharmacodynamics in vivo. The power of PET rests in the ability to incorporate radionuclides such as ^{18}F and ^{11}C into drugs and detect tissue-penetrating gamma emissions that arise from positron annihilation. Carbon-11 is a compelling radionuclide for incorporation because carbon is ubiquitous in organic molecules; hence, its use does not change the pharmacological properties of the drug. The use of ^{11}C in PET; however, has been often limited by its 20.4 min half-life. As such, we investigated a reaction to directly incorporate the immediate cyclotron product $^{11}\text{CO}_2$ into functional groups via an organocatalytic approach. Hindered organic amines are effective catalysts for this method as they have been shown to react in equilibrium with CO_2 , thus activating carbon dioxide and potentially enabling the formation of carbamates and carbonates. Optimal conditions for forming the carbamate and carbonate functional groups directly from CO_2 were investigated by screening solvents, bases, base concentrations and temperatures in

order to promote zwitterionic base- CO_2 equilibria in solution. Carbon dioxide retention and release rates in solution were determined by tracking $^{11}\text{CO}_2$. 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) was the most effective base for trapping CO_2 in solution at room temperature, trapping on average 5–6 times better than 4-dimethylaminopyridine (DMAP) or 1,4-diazabicyclo[2.2.2]octane (DABCO). Acetonitrile was the optimal solvent for CO_2 retention. ^{13}C -NMR analysis of the DBU- CO_2 complex in MeCN indicated the presence of dissolved CO_2 ($\delta=124.8$ ppm). ^{13}C -NMR analysis of DBU- CO_2 in DMSO lacked the carbamate ($\delta=160.7$ ppm) and CO_2 resonances, possibly suggesting a fast transition between the two species in low concentration. The carbamate functional group was formed (yields=20%) by reacting DBU, CO_2 and fluorobenzylamine at 50 $^\circ\text{C}$, and then adding benzyl bromide to all at 0.28 M concentrations. The reaction, however, is not optimized for the formation of carbamate. Further studies are needed to determine optimal equilibrium conditions that favor carbamate formation and minimize the production of by-products.

*** Attempts to Minimize Excess CO_2 in Earth's Atmosphere Using Ruthenium-Compound**

Misbah Howard and Mickdy Milien (KINGSBOROUGH COMMUNITY COLLEGE, BROOKLYN, NY 11235), Dr. Varattur Reddy (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

Although carbon dioxide (CO_2) is a greenhouse gas essential to maintaining the temperature of Earth, an excess of it can raise Earth's temperature to lethal levels. In order to develop a chemical solution in which we can chemically reduce CO_2 , we synthesized a possible catalytic compound, ruthenium glucal (Ru-glu). Ru-glu has the potential to act as a catalyst because of the two hydride ions (H^-) that it possesses. In order for a reduction to take place, we need Ru-glu to donate these (H^-) to CO_2 . However, we first wanted to see if Ru-glu could transfer (H^-) to the two known hydride acceptors, triphenyl carbenium cation, BF_4^- (trityl); and n-benzyl nicotinamide, PF_6^- (NBN). If Ru-glu transferred hydrides to both trityl and NBN, we knew it was possible to do the same for CO_2 . In each case we used spectroscopic and analytical techniques to determine the possibility of Ru-glu transferring a hydride ion to these compounds. When we mixed Ru-glu with trityl, the UV spectrum showed that it reacted very quickly; whereas, in the reaction between Ru-glu and NBN, the NMR showed that the hydride transferred only after heating the solution at 80 $^\circ\text{C}$. Since there was a hydride transfer from both reactions, carbon dioxide was bubbled into a solution of Ru-glu for four hours at 80 $^\circ\text{C}$. Ru-glu transferred a hydride ion to CO_2 , chemically reducing it into a formate complex. This clearly demonstrated that Ru-glu reduces carbon dioxide and can therefore be a solution for eliminating this excessive greenhouse gas.

High-Performance Liquid Chromatography Separations of Biological Molecules Using Microfluidic Chips Packed with Silica Particles and Porous Polymer Monoliths.

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Micro biological technologies today require direct injection of an analyte, fast mass transfer and real-time detection integrated into a single device. Poly(styrene-co-divinylbenzene) monoliths were prepared in situ in microfluidic polyimide HPLC chips via thermally-initiated free-radical polymerization and used as the stationary phases for HPLC separation. The chips, featuring a 200 μm cross-section, enable the minimizing of dead volumes and band broadening. Rapid baseline separations of proteins, peptides and protein digests at nanomolar concentrations were achieved with the monolithic stationary phases. Compared to chips packed with porous silica particles, the monolith affords better separations for larger molecules. These microfluidic chips can be used in proteomic analyses and can thus be adapted for biosecurity devices.

Hydrogen Production by Ethanol Steam-Reforming Over Supported Cobalt and Cobalt-Zinc Catalysts

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Ethanol steam-reforming (ESR) is considered a promising alternative for hydrogen production that can be employed as a renewable and environmentally friendly source of energy. In this research, ESR was studied over several zinc oxide and zirconium oxide supported cobalt and cobalt-zinc catalysts such as 10% Co/ZnO-Na, 10% Co/ZrO $_2$, 10% Co 5% Zn/ZrO $_2$, 10% Co 1% Zn/ZrO $_2$, to evaluate their catalytic performance and to determine the effect of cobalt-zinc interactions in altering the ratio of Co_2^+ to Co_0 during the steam-reforming reaction. Sodium promoted cobalt-zinc oxide catalyst, Co/ZnO-Na, was prepared by co precipitation of aqueous solutions of Zn (NO_3) $_2$ and Co(NO_3) $_2$

followed by addition of aqueous Na_2CO_3 at 313K. Co/ZrO_2 was prepared by impregnation of ZrO_2 support by an aqueous solution of $\text{Co}(\text{NO}_3)_2$. Co-Zn/ZrO_2 catalysts were prepared by co-impregnation of ZrO_2 by aqueous $\text{Co}(\text{NO}_3)_2$ and $\text{Zn}(\text{NO}_3)_2$ solutions. The prepared catalysts were dried at 383K overnight, crushed into granules of 65–100 mesh and calcined in air at 623–773K for three hours. All catalysts were characterized by Bruner Emmett Teller (BET) surface area and pore volume measurements, temperature-programmed reduction (TPR), hydrogen chemisorption and X-ray diffraction (XRD) measurements. The catalysts were tested for activity and selectivity for ESR using a plug flow reactor with a reagent feed consisting of a gaseous mixture of ethanol, water and nitrogen at 723K. Prior to testing, each catalyst was reduced for two hours with 10% H_2 in N_2 at 723K. Among the various catalysts tested, Co-Zn/ZrO_2 catalysts exhibited higher CO_2 selectivity (77%) and low CH_4 selectivity (6.5%) at low ethanol conversion (9%). These results demonstrate that with appropriate modifications in catalyst preparation and reaction conditions, Co-Zn/ZrO_2 catalysts can be used for efficient production of H_2 from ethanol steam-reforming.

Ni/NiO Core/Shell Nanoparticles for Information Storage Applications

Lauren Kreno (Cornell University, Ithaca, NY 14850), Stanislaus S. Wong (Brookhaven National Laboratory, Upton, NY 11973). In the quest for sophisticated magnetic materials, core/shell nanoparticles present a compact medium for data storage. Specifically, an antiferromagnetic metal oxide shell covering a ferromagnetic metallic core traps some of the core's magnetic spins at the metal-metal oxide interface, creating a detectable magnetic signal. To explore this system, monodisperse transition metal nanoparticles were synthesized using a modified polyol process. Subsequently, the particles were subjected to various oxidation treatments to induce the growth of metal oxide on the surface of the particles. Evaluation of the oxidation products showed that heat treatment in air yields the most control over particle oxidation. The temperature of the heat treatment was then varied to regulate the oxidation of the particles, which, along with particle size and morphology, was monitored using powder X-ray diffraction and transmission electron microscopy. Analysis of the particles using a superconducting quantum interference device revealed that the extent of oxidation affects the particles' magnetization and the magnitude of the observed exchange bias. By producing monodisperse metal nanoparticles and establishing a protocol to control their oxidation, it was possible to study trends in the particles' exchange biases, essential properties for magnetic storage materials.

Characterization and Durability Analysis of a-SiC:H as a Protective Layer for a Multi-Junction a-Si:H Tandem Cell for Use in Photoelectrochemical Hydrogen Production

Leah Kuritzky (Stanford University, Stanford, CA 94305), Todd Deutsch (National Renewable Energy Laboratory, Golden, CO 80401). The current crisis in fossil fuels energy sources and rising CO_2 levels in the atmosphere are creating increasing demand for renewable and carbon-free energy supplies for the 21st century. A hydrogen economy is one vision for the future if it can be realized via efficient electrolysis of water. This investigation seeks a photoelectrochemical (PEC) cell that will directly convert water to hydrogen and oxygen without the losses associated with the current method of solar hydrogen generation, photovoltaic-electrolysis. The material, hydrogenated amorphous silicon carbide (a-SiC:H) thin film, was investigated for use as a photoelectrode and also as a protective layer on a multi-junction amorphous silicon (a-Si:H) tandem cell. The band gap of a-SiC:H was measured using photocurrent spectroscopy. Indirect and direct transitions were found at 1.72 eV and 1.98 eV respectively, and both are within the range for unbiased water-splitting. The flat band potential was measured for a-SiC:H using photocurrent (PC) onset and illuminated open-circuit potential. Both methods showed that the flat band potential lies negative of the oxygen redox potential, therefore requiring an external bias to split water. A single junction a-Si:H/a-SiC:H monolithic tandem solar cell was able to provide the needed bias to correct for the energetics, placing the flat band potential positive of the oxygen redox potential. This tandem cell also provided a 800–900 mV positive shift in PC onset for both two and three electrode configurations and an average short circuit current density of $-1.3 \times 10^{-8} \text{ A/cm}^2$. Durability tests lasting 24 hours were done on a-SiC:H to evaluate the stability of this material in pH 2 electrolyte under illumination with a constant applied current density. Samples of both glass/Mo and stainless steel/Mo showed improved PC response after the 24 hour test, which may be due to internal passivation of dangling bonds facilitated by the applied bias. Additionally, HF etches were performed to investigate the effect of the native oxide layer on durability. The HF

etches temporarily improved the PC response, with PC onset shifting by 0.23 V, but after 67 hours of re-exposure to air, and presumably, re-growth of the oxide, the PC response returned to pre-etch levels. The overall results of characterization and durability testing of these materials are promising and substantiate the potential of a-SiC:H to split water with the bias provided by an a-Si:H tandem cell.

*** Novel Technique of Carbon Dioxide Capture from Flue Gas of Coal Power Plants**

Richard Lester (College of DuPage, Glenn Ellyn, IL 60137), Yupo Lin (Argonne National Laboratory, Argonne, IL 60439). Over 50% of the electrical power in United States comes from coal burning power plants. During the production of electricity waste gas is released through a flue. The flue gas contains 15% of CO_2 (bi-carbonate) and other gases such as sulfur dioxide and nitrous oxides. The CO_2 being produced may be a contributing factor to global warming. The objective of this project is to develop advanced separation technology to capture majority of CO_2 in the flue gas before it is released into the atmosphere. The innovative technology should have much better capture efficiency, have lower energy consumption and be cost effective compared to current practices such as the use of pressure and amines. The amine technology only captures up to 20% of the CO_2 and could increase the overall cost of electricity production by 89%. The new technology under development is based on Argonne National Laboratory's proprietary resin wafer electro dialysis (ED). In this technology, CO_2 gas is fed into the ED and captured in aqueous phase enhanced by biological catalyst. The captured CO_2 in the aqueous phase then could be released into a controlled environment. The release of CO_2 is also enhanced by a similar biocatalyst. The amount of dissolved CO_2 in the collected samples is determined in terms of carbon using a total organic carbon analyzer. The capture/release efficiency of CO_2 is evaluated by changing operating parameters of the ED bioreactor. The results of this experiment have proven the concept of using a ED bioreactor to capture and release the CO_2 gas. However, there are still many variables to consider and test. Further research is needed to optimize CO_2 capture and release efficiency.

Investigating the Toxicity of Pyridinium and Imidazolium Ionic Liquids

Xing Li (Queensborough Community College, Bayside, NY 11364), James F. Wishart (Brookhaven National Laboratory, Upton, NY 11973). Ionic liquids (ILs) are salts with melting points below 100 degrees Celsius. Much attention has been drawn to ILs lately because of their relative non-volatility, non-flammability, wide liquid range and high conductivity. These properties make ILs very good candidates as solvent alternatives to volatile organic solvents, but there is absence of adequate toxicity data. This work evaluates a series of imidazolium and pyridinium ILs for their toxicity to a variety of microorganisms. The effect of purity based on color, branching of the alkyl chain and identity of the anion was investigated. Halide salts based on 1-methylimidazole and pyridine were prepared with branched and unbranched alkyl halides of varying chain lengths. These salts were purified and converted to ILs bearing the phosphate and bis(trifluoromethylsulfonyl)imide anions. These liquids were prepared in different grades of purity by varying the temperature of the halide salt synthesis. The structures of the salts were confirmed using ^1H , ^{13}C and ^{31}P Nuclear Magnetic Resonance (NMR) spectroscopy. The grades of purity were evaluated using Ultraviolet-visible spectroscopy (UV-Vis) spectroscopy. The liquids were screened for their toxicity to a variety of organisms including bacteria (*Bacillus subtilis*, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Klebsiella pneumoniae*); mold (*Rhizopus stolonifer*) and mosquito larvae. Preliminary results indicate that bacterial growth inhibition caused by ILs is dependent on concentration, alkyl chain length and bacterial strain. From our preliminary results, color does not appear to have an effect on toxicity.

Semiconductors and Scintillators

Peter Liu (Ohlone College, Fremont, CA 94539), Dale L. Perry (Lawrence Berkeley National Laboratory, Berkeley, CA 94720). Scintillators reflect X-rays and emit the visible light that is proportional to the X-ray energy. Researchers at Lawrence Berkeley National Laboratory are producing new scintillators to improve the field of radiation detection. Pulsed laser deposition is the most effective method to produce thin films. X-ray diffraction and scanning electron microscopes can help scientists characterize any thin film. The pulsed laser deposition created a thin film from lanthanum chloride (LaCl_3) powder. The X-ray diffraction instrument confirmed the identity of LaCl_3 . The scanning electron microscope was used to view the images of LaCl_3 powder. Also, they made a few targets of LaCl_3 . The LaCl_3 film made with ZnO turned out to be a better target because it is not hygroscopic. Under the scanning microscope, the surface of the LaCl_3

powder turned out to be uneven. The precise amount of pressure is essential to make a target for any inorganic compound.

Photochemical Modification of Silica-Based Monoliths with Nanolayer of Fluorinated Methacrylate

Joao Luna (BARRY UNIVERSITY, MIAMI SHORES, FL 33161), Frantisek Svec (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). Stationary phases for micro liquid chromatography (μ LC) with a nanolayer of fluorinated methacrylate have been prepared inside of ultraviolet (UV) transparent capillaries via photoinitiated grafting of fluorinated polymer onto the pore surface of a porous silica monolith. In-situ free radical grafting polymerization of pentafluoropropyl methacrylate on the pore surface of silica was initiated at 110 °C followed by 5 min exposure to UV light. Scanning electron microscopy (SEM) was utilized for the evaluation of the skeletal structure of the prepared monoliths. Formation of the desired fluorinated layer was confirmed utilizing μ LC with separation of a model mixture of compounds consisting of polar and non-polar analytes. Successful photografting of fluorinated nanolayer on a porous silica surface was accomplished in 8 min in the presence of benzophenone. Chromatographic separation of thiourea, ethylbenzene and hexylbenzene was achieved in less than 4 min using simple isocratic conditions. These results show the potential of silica monoliths grafted with a nanolayer of fluorinated functional groups as a suitable column for reversed-phase liquid chromatography. A combination of thermal and UV initiated grafting represents fast and simple approach of surface modification and has a potential of becoming an attractive alternative to thermal preparation of functionalized separation media.

Application of Palladium Catalyzed Decarboxylation in Organic Synthesis and in the Production of JP-8 Jet Fuel

Justin Mallek (UNIVERSITY OF WISCONSIN-MADISON, MADISON, WI 53706), George Kraus (AMES LABORATORY, AMES, IA 50011). A highly selective palladium catalyzed decarboxylative reaction that converted carboxylic acids into olefins was explored. This little-used reaction could be employed to produce the military jet fuel JP-8. Current biodiesel is produced from triglycerides which are harvested from oil-rich crops. The benefit of biodiesel is that it is a widely available, renewable resource. The problem is that it can congeal at low temperatures, rendering it useless as a jet fuel. By catalytically removing the carboxylic acid, this reaction will produce long chain alkenes very similar to the currently used JP-8 fuel. The method for this reaction requires the use of inexpensive anhydrides to convert the carboxylic acid to a mixed anhydride. Bis(2-(diphenylphosphino)phenyl) ether is coordinated with palladium chloride to form the catalytic complex in situ. Decarboxylation occurs overnight at a temperature of approximately 120 °C. During the examination of this reaction, the formation of alpha-olefins has been confirmed and the experimental protocol was successfully standardized. Using the CEM Discover microwave reactor, a 70% yield of 1-undecene was achieved after only five hours of heating to 120 °C. This reaction was also used successfully in the decarboxylation of diphenylacetic acid to diphenylmethane in 62% yield.

Polonium-Lead Separations to Determine the Best Method for the Quantification of Clean Lead for Use in Low-Background Detectors

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Very sensitive detectors are used for low-background applications including the detection of environmental radioactivity, double-beta decay and dark matter. In order to reduce the background noise enough to utilize the sensitivity of these detectors, lead with little or no alpha activity is required to form the shielding. In the past, antiquity lead shielding was used for low-background detectors because lead's most prominent alpha-emitting isotope, ^{210}Pb , has a short half-life. The microelectronics industry is also greatly affected by alpha activity in lead and solder and has begun producing "clean" lead for purchase. To quantify how clean the available lead is, ^{210}Pb and, during procedural experiments, a ^{209}Po tracer must be physically or chemically removed from the bulk lead. A reliable procedure for chemical separations that does not use large volumes of ultra-high-purity chemicals has not yet been established. Lead was dissolved and a known amount of ^{209}Po tracer was added. The samples were put through each of two new procedures. The first procedure was based on complete dissolution of the lead followed by a column separation. The second method investigates the utility of a pre-separation step using precipitation of the lead prior to column separation. The resulting solutions were run through strontium resin columns from Eichrom Inc., a United States Transuranium and Uranium Registries (USTUR) electrodeposition procedure, and scheduled to be alpha counted for a minimum of three

days. Though neither of the tested procedures had acceptable logistics for large scale implementation, later alpha counting showed which procedure is more promising for further development.

*** [^{18}F]Fluorobenzoquinone for Peptide and Protein Labeling**

Elizabeth Millings (SUFFOLK COUNTY COMMUNITY COLLEGE, SELDEN, NY 11784), Jacob M. Hooker (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Fluorine-18 radiotracers for positron emission tomography (PET) have facilitated medical imaging studies of the brain and provided useful information about biochemical processes. Labeling and subsequent imaging of proteins and peptides can be particularly informative as they offer the ability to target specific cell and tissue types. The 109.7 min. half-life of F-18 and the low concentrations at which radiochemical reactions are conducted preclude previously used synthetic methods. Moreover, these methods are often long, requiring many steps and resulting in low yields. We set out to develop a simple and efficient way to incorporate F-18 into peptides and proteins using [^{18}F]fluorobenzoquinone (FBQ). The electrophilic nature of quinone functional groups makes them ideal "bridges" by which proteins and [^{18}F]fluoride, both nucleophiles, can be ligated. Envisioning a simple, one-step synthesis of [^{18}F]FBQ, we began by screening reactions of chlorobenzoquinone (CBQ) with [^{18}F]fluoride salts under various conditions. The optimal combination of cation, solvent and temperature was determined by High Performance Liquid Chromatography (HPLC) and Thin-Layer Chromatography (TLC) analysis. Reaction of CBQ with cesium fluoride in acetonitrile (MeCN) at 80 °C afforded FBQ in up to 40% yield. The major product of the reaction was coincident with an authentic sample of FBQ, which was prepared according to the literature and verified by ^1H , ^{19}F and ^{13}C -NMR spectrometry. Initial attempts to incorporate [^{18}F]fluoride prior to reaction optimization were unsuccessful, however the results improved when MeCN was used as a solvent instead of dimethyl sulfoxide (DMSO). Continued screening of cation, basicity and concentration afforded a stable radiochemical yield of 2–6% by radioactive TLC analysis. Future work will focus on increasing the yield by investigating quinone starting materials with other leaving groups, for example, iodoquinone. Following isolation and purification, [^{18}F]FBQ reactivity with various proteins and peptides will be determined to find optimal conditions for labeling.

Detection of Plant Growth Hormone Indole-3-Acetic Acid Using Gas Chromatography Mass Spectrometry (GC-MS)

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The need for alternative transportation fuels, such as ethanol, is an increasingly important global issue as gasoline prices rise and reserves dwindle. To effectively produce alternative fuels from biomass, it is essential to understand plant metabolism and growth. One important part of the research into ethanol production from biomass is the implementation of analytical methods to investigate plant metabolites to find the limit of detection and quantification of the plant growth hormone indole-3-acetic acid (IAA), commonly known as auxin. Gas Chromatography/Mass Spectrometry (GC-MS) was used to study IAA produced by plants, and by endophytic microbes in plant growth media. Leaf samples were cryomilled and extracted with acidified isopropanol and labeled ^{13}C IAA was added as an internal standard. Once grown to a uniform cell density, the bacterial growth medium was freeze-dried and extracted in the same manner as the plant matter. The resultant extracts of leaf and bacterial growth medium were then isolated using a C_{18} Sep-Pak column. The hormone extract was silylated with N-methyl-N-trimethylsilyltrifluoroacetamide (MSTFA)+1% trimethylchlorosilane (TMCS), and analyzed. IAA standards were analyzed and the hormone was detected consistently at 4 ug/ml. A reliable standard curve could not be generated from the prepared standards due to erratic data between sample runs ($R^2=0.8814$), therefore no limit of quantification could be determined. IAA was not detected in plant or bacterial samples, therefore IAA levels must be less than 20 ug/g DW based on 4 ug/ml limit of detection. Solubility of the plant and bacterial was low adding a source of potential error. Future work within this group includes inoculation of poplar cuttings with bacteria to monitor plant growth and hormone levels, analysis of the high nutrient bacterial growth media, continued analysis of various plant samples by GC-MS, and further troubleshooting of the instrument to determine the cause of the lack of repeatability.

Surfactant-Templated Synthesis of Amorphous Nanoporous Metal-Phosphates for Use in Secondary Batteries

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Lithium ion secondary batteries contain crystalline materials that undergo phase transitions when charging and discharging. Intercalation of lithium ions causes sheer stress within the crystalline material which leads to fracturing. Decreased battery life and energy storage are results of crystal lattice fracturing. Amorphous, nanoporous materials that could replace crystalline materials would undergo less sheer stress and enable batteries to store more energy and last longer. Amorphous, nanoporous metal-phosphate materials can be synthesized using surfactants as a template for synthesis. The metals chosen for this study include vanadium, tin, manganese, cobalt and iron. These metals were complexed to phosphate ions using cationic surfactants under ambient conditions. X-ray diffraction, surface area analysis and scanning electron microscopy were used to characterize the materials as amorphous and nanoporous. Three novel amorphous materials were formed which show increased porosity over crystalline materials of the same chemical composition. These novel metal-phosphate materials display amorphous or porous characteristics which have been shown to perform well as cathodes or anodes in secondary batteries. Additionally, two novel clay-like structures were formed which, although not amorphous or porous, may perform well as battery cathodes due to increased spacing between sheets within the material. Battery performance testing is forthcoming to test the ability of these materials to convert, store and utilize energy.

Thermochemical Transformations in $2\text{MNH}_2\text{--}3\text{MgH}_2$ Systems (Where M=Li or Na)

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Related to the need of high capacity hydrogen storage materials, there is a growing interest in lightweight compounds such as lithium- or sodium-based hydrides. Among them, metal-nitrogen-hydrogen (M-N-H) systems have been regarded as among the most attractive materials. Hydrogen storage potential of $2\text{MNH}_2\text{--}3\text{MgH}_2$ systems (where M=Li or Na) was investigated using pressure composition temperature (PCT), residual gas analysis (RGA) and X-ray powder diffraction analysis (XRD). Samples were thermally dehydrogenated by heating from 25 °C to 395 °C at a heating rate of 1 °C/min. Analysis of the final products showed formation of magnesium nitride, alkali metal hydrides and pure hydrogen after the heating of the mixtures. Amount of released hydrogen is 6.5 wt% for the $2\text{LiNH}_2\text{--}3\text{MgH}_2$ system and 5.1 wt% for the $2\text{NaNH}_2\text{--}3\text{MgH}_2$ system. The overall reaction can be presented as: $2\text{MNH}_2(\text{s}) + 3\text{MgH}_2(\text{s}) \rightarrow \text{Mg}_3\text{N}_2(\text{s}) + 2\text{MH}(\text{s}) + 4\text{H}_2(\text{g})\uparrow$. Hydrogen release was observed starting at 190 °C in a lithium system and at 140 °C in a system with sodium. It was found that minor ball milling improves thermal properties of mixtures due to decreased particle size and increased number of defects. RGA analysis of released gas showed formation of pure hydrogen in both systems. Final products of our experiments agree with the research done by Dolotko and Pecharsky using a mechanochemical transformation procedure of these systems. Heating of mixtures to different temperatures allowed us to investigate formation of intermediate compounds during reaction. It was observed that the intermediates formed depend on the transformation method employed. To gain a more complete understanding of this system, future research should include a detailed investigation of the mechanism of these transformations using alternative heating temperatures, solid state nuclear magnetic resonance (NMR) and other techniques.

Improving the Luminescent Properties of Titanium Dioxide Nanoparticles

Marina Poluektova (UNIVERSITY OF ILLINOIS, URBANA-CHAMPAIGN, URBANA, IL 61820), Tijana Rajh (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). Previous research has shown that titanium dioxide (TiO_2) nanoparticles linked to specific antibodies can be used for photodynamic therapy to selectively destroy cancer cells. A study of the mechanism of the lysis of the cancer cells could be done by imaging cells with TiO_2 nanoparticles with a confocal laser scanning microscope such as the Zeiss LSM 510 used for this experiment. A confocal microscope produces an image of the sample based on its fluorescence and allows for the creation of three dimensional images, an advantageous option which would allow the detection of the location at which cell lysis occurs within the cells. However, TiO_2 nanoparticles do not exhibit fluorescence strong enough to successfully monitor the particles by use of a confocal laser scanning microscope. Based on previous experiments, it has been proposed that titanium dioxide becomes more luminescent after exposure to X-rays. TiO_2 nanoparticles in solution at a concentration of 0.0775 M were examined with the LSM 510 before and after the exposure to X-rays in the Bruker analytical X-ray source. A conclusion was reached that the analytical source was

not powerful enough to enhance TiO_2 luminescence as no significant increase in fluorescence was detected. When TiO_2 nanoparticles were bound to IgG antibodies marked with fluorescein isothiocyanate (FITC), an increase in fluorescence was observed which was about 2.5 times greater at the 400 dopac coverage of the surface of TiO_2 nanoparticles than at the 100 dopac coverage. In the samples of TiO_2 attached to fluorescein with and without dopamine surface modification, the presence of dopamine quenched the fluorescence. Enhancement of fluorescence was only visible at a pH of 6.1, although a greater fluorescence was expected at a pH of 7.4.

The Origin of Fluorescence in PAMAM Dendrimers

Julia Price (UNIVERSITY OF TENNESSEE-KNOXVILLE, KNOXVILLE, TN 37996), Kunlun Hong (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Dendrimers are synthetic macromolecules with highly regular three-dimensional architectures with a unique combination of intrinsic properties such as the presence of interior cavities, monodisperse nano-sized structure and chemical uniformity. Though many kinds of dendrimers have been investigated, polyamidoamine starburst dendrimers (PAMAM) with ethylenediamine (EDA) cores are one of the most studied due to their non-immunogenicity and biocompatibility, making them candidates for biological applications. Recently it has been found that PAMAM shows intrinsic fluorescence, which contradicts classic theory. It is generally accepted that the fluorescence signals of molecules usually originate from aromatic structural units. However, to date, this unique photoluminescence property in PAMAM has not been investigated. In our study, the fluorescence behavior of generation 4 (G4) PAMAM was studied. Samples of G4 PAMAM in H_2O , D_2O and a tertiary amine-terminated G4 in D_2O were prepared at varying pH levels. The pH was measured throughout to ensure stability. Absorbance spectra were collected from a UV-Vis spectrometer and emission and excitation spectra were collected from a FluoromaxP spectrometer over a two week period. Emission was more significant in lower pH solutions because quenching of primary amine groups was lessened. Solutions in H_2O had higher absorbancies than counterparts in D_2O , which indicated that hydrogen bonding plays a major role in the fluorescence behavior. This is because hydrogen bonding in H_2O is more significant than it is in D_2O . However, side reactions, such as oxidation, likely occur as well. Currently, we are studying PAMAM dendrimers with other functional groups to determine if their fluorescent properties are related to surface terminal groups. In addition, we are also testing the role of oxidation in the fluorescence behavior in PAMAM dendrimers. The origins of the fluorescence behavior of PAMAM dendrimers seems to be more complicated than previously thought.

Oxygen-Tolerant Anodic Electrocatalysts for Polymer Electrolyte Fuel Cells

Tyler Qiu (UNIVERSITY OF CHICAGO, CHICAGO, IL 60637), Xiaoping Wang (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). Some major barriers preventing the commercialization of polymer electrolyte fuel cells (PEFC) as highly effective alternative energy sources are the cost and degradation of the platinum-based electrocatalyst layers used in both the cathode and anode of PEFC. The purpose of this project is to develop alternative anode electrocatalysts that do not contain platinum yet still provide at a lesser cost, comparable hydrogen oxidation activity to that of platinum-based catalysts and be more inert to oxygen reduction. The non-platinum catalysts studied were bimetallic gold-based nanoparticles supported on high surface area carbon. The catalysts were prepared by impregnation and post reduction at elevated temperatures and subsequently made to inks that were applied onto a rotating disk electrode (RDE) to form thin-film RDE catalysts. Cyclic voltammetry (CV) and the RDE techniques were used to evaluate the hydrogen oxidation activity of various gold bimetallic systems. The activity of the bimetallic catalysts were then normalized and compared to commercial platinum-based catalysts. Preliminary results show that the hydrogen oxidation activity for gold bimetallic catalysts depends on the identity and molar ratio of the second metal. While some of the gold bimetallic systems showed significantly lower activity, the 3:1 gold of the second metal exhibited an activity comparable to that of the commercial platinum catalyst. Expected results from further experimentation will determine the optimum molar ratio of gold to the second metal and also determine which bimetallic system provides the greatest activity and oxygen tolerance.

Investigation of Factors Affecting Analyte Desorption in Desorption Electrospray Ionization Mass Spectrometry

Andrew Rajczewski (RENSSELAER POLYTECHNIC INSTITUTE, TROY, NY 12180), Gary Van Berkel (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Desorption Electrospray Ionization Mass Spectrometry (DESI-MS) is a newly-developed atmospheric pressure and surface sampling/

ionization technique that offers the sensitivity and selectivity of mass spectrometry with minimal sample preparation. These qualities make it ideal for use in forensics, pharmacology, etc. Currently there has been scant investigation of the factors influencing analyte desorption in DESI-MS. The focus of this research was to explore factors affecting desorption of alkylammonium salts from high-performance thin-layer chromatography (HPTLC) plates in DESI-MS and to compare these data with desorption of analytes in electrospray mass spectrometry (ES-MS). The effects of alkyl chain length, molecular diameter and shape on desorption efficiency were investigated. The influence of alkyl chain length on desorption effectiveness was examined via a series of linear alkylammonium salts of increasing alkyl chain length; the effect of diameter was examined using a series of spherical alkylammonium salts of increasing diameter. To examine the influence of shape, alkylammonium salts of identical mass but with shapes ranging from spherical to linear were analyzed and compared. In the experiments, samples of analyte were spotted onto normal (hydrophilic) and reverse-phase (hydrophobic) HPTLC plates and analyzed with DESI-MS. Acetonitrile, methanol, water and mixtures thereof were used as spray solvents. It was found that desorption is most effective when the spray solvent is acetonitrile, and least effective when water or methanol is used. In general, the linear alkylammonium salts show increasing desorption effectiveness with increasing alkyl chain length under all but aqueous conditions, potentially due to a surfactant effect in aqueous solvents and a solubility effect in organic solvents. The spherical analytes behave similarly to the linear analytes on the normal phase, but no obvious pattern was seen on the reverse-phase plates. Spherical analytes desorbed more effectively than linear analytes under all but aqueous conditions. In ES-MS tests, shape trends are similar to those seen in DESI-MS, although the linear and spherical alkylammonium salts show greater desorption with methanol as a spray solvent. These data suggest that DESI-MS desorption can be optimized in chemical analyses; however, further testing of possible matrix effects and desorption on other media is needed before industrial applications can be undertaken.

Synthesis of Porous Alumina Monoliths for Applications in Microscale Liquid Chromatography

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The in situ synthesis of the alumina-based monoliths within 50–100 μm ID fused silica capillaries via the sol-gel method has been studied. It was possible to prepare porous alumina monoliths from a mixture of aluminum nitrate nonahydrate, acetonitrile, methanol, N-methylformamide and propylene oxide. Evaluation of structural characteristics was performed by means of optical microscopy, scanning electron microscopy and nitrogen adsorption analysis. Monoliths were synthesized with porous skeleton, surface area of 29 m^2/g and a predominant average pore size of 170 nm. The chromatographic performance of the alumina-based monoliths was investigated under isocratic conditions using a microscale liquid chromatography. Separation of a mixture of imidazole and pyrazole was achieved in less than 2 min and a binary mixture of hexylbenzene and thiourea was separated in less than 40 s. The backpressure analysis performed using $\mu\text{-LC}$ has shown that the structures are permeable to fluids and that they can withstand pressures as high as 230 bar.

Silicon Nitride for Semiconductor Photoelectrochemical Water Splitting

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Silicon nitride was analyzed to determine if it is an effective material to split water in direct photoelectrolysis application. Band gaps determined via photocurrent spectroscopy were found to exhibit indirect transitions between 1.45–1.85 eV. Some of the higher SiN band gaps fall within the optimal band gap range for direct photoelectrolysis (1.6–2.2 eV). Flat band potentials were not negative enough to drive the hydrogen evolution reaction for these n-type films. Silicon nitride is therefore ineffective as a direct photoelectrolysis device, because its band edges are not aligned with respect to the redox potentials, a criterion necessary to generate hydrogen from water splitting. Twenty-four hour durability tests in 1M KOH revealed that this material is highly unstable, most likely due to substrate adhesion difficulties. The n+Si/i-SiN junction materials did not generate higher currents than the i-SiN samples. This is most likely due to pinholes and corrosion sites on the surface of the semiconductor. High quality and more uniform depositions need to be grown in order to fully conclude n-i-junction behavior. Overall, SiN exhibits an optimal band gap but does not

have ideal band edge alignments and does not last long in electrolyte solution. Therefore it does not appear to be a valid candidate for photoelectrochemical water splitting.

New Synthesis Routes to Iron-containing Lithium Metal Oxides and Phosphates for Lithium Batteries

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The objective of this project is to develop and optimize new synthetic routes and methodologies to incorporate iron into cathode materials for lithium batteries. The introduction of increased amounts of iron into electrode formulations could potentially yield lower cost, more passively safe batteries that are environmentally friendly and recyclable. In addition, the large abundance of iron as a transition metal in the earth crust would be critical for supplying the growing demand for large batteries to supplement power for hybrid electric (HEV), plug-in electric (PHEV), and eventually electric vehicles (EV) recharged on the grid. To meet these objectives, unary, binary and tertiary Fe, Mn and Ni hydroxide-type precursor battery materials were synthesized in a nitrogen atmosphere to avoid air oxidation. Various reaction conditions such as solvent choice, pH, temperature of reaction, speed of reaction and additives have been used as a way to modify the compositions, electrical conductivity, surface properties and morphological character of the products. Samples were divided to produce final lithium metal phosphates, lithium metal oxides and composites of both members for use as battery electrodes. Characterizations were performed using X-ray Diffraction (XRD) and Scanning Electron Microscope (SEM) to analyze the various materials' phase purities and morphologies. Materials were processed into electrode laminates, built into coin cells and tested on a battery cycler. Work in this area is ongoing and results and conclusions will be obtained after tests and characterization is completed.

Electrochemical Effects of Novel Transparent Conductive Coatings Deposited on p-GaInP₂ for Photoelectrochemical Water Splitting

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We report on the electrochemical effects of novel transparent conductive coatings deposited at various thicknesses (0, 5, 10, 15 and 20 coats) on the surface of p-GaInP₂ to assess the impact of these coatings on the photoelectrochemical (PEC) splitting of water into hydrogen and oxygen. PEC hydrogen production promises to be a renewable, domestic, non-polluting and efficient way of storing the sun's energy for subsequent conversion to electricity via hydrogen fuel cells. The coatings chosen for study are thought to be endowed with the right properties so as to both protect the surface of p-GaInP₂ from degradation in aqueous media and favorably vary the material's interfacial kinetics and energetics. Mass spectrometer measurements of flatband potential (V_{fb}) provided the most promising results overall, showing a direct relationship between positive V_{fb} shifting and the number of novel coatings deposited on the p-GaInP₂ samples. Band edge shifts in the correct direction were sometimes enough to achieve sufficient band edge overlap for PEC water splitting. This promising trend, however, was challenged by the open circuit photovoltage (OCP) and photocurrent onset V_{fb} determinations, each of which showed little or no obvious difference between the V_{fb} values of the coated and uncoated samples. Photocurrent magnitude and onset measurements indicated little to no effective charge transfer catalysis provided by the coatings. The former technique suggested that the coatings may actually be attenuating light to some degree. Lastly, durability analyses failed to show enhanced stability and performance of the coated p-GaInP₂ samples with respect to the uncoated controls. Future work will predominantly focus on optimizing the newly developed, aggressive process of manufacturing and treating the coatings, which may be destructive to the underlying p-GaInP₂.

Analysis of CuGaSe₂ Films for Photoelectrochemical Water Splitting

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Energy is a pressing issue due to industrial nations' dependence on finite and harmful hydrocarbon fuel sources and the increasing demand for these fuels by rising nations. A viable alternative to hydrocarbon energy is the energy harnessed in hydrogen. Hydrogen can be produced using renewable resources such as water and solar energy using photoelectrochemical (PEC) cells. A semiconductor that could be used as the photocathode in a PEC cell is CuGaSe₂ (CGS). This material's PEC characteristics were evaluated including the band gap, flat band potentials and ability to generate hydrogen under illumination. The techniques used to determine these properties include photocurrent

spectroscopy, illuminated open-circuit potential measurements, and chopped light current-potential measurements, respectively. The band gaps were determined to be around 1.6 eV and the flat band potentials were too negative to split water. A standard platinum treatment was then performed on the CGS in an attempt to increase the photocurrent. Parameters including the Coulombic density of platinum deposited, duty cycle, light intensity and electrolyte composition during the platinum electrodeposition were varied. A colloidal platinum treatment was also done by soaking the electrodes in water containing platinum colloids. The standard platinum treatment did increase the photocurrent of the CGS, however, the only varied treatment that produced consistent positive results was the treatment with increased light intensity during deposition. The colloidal treatment also gave consistent positive results. This is probably due to the neutral environment during electrodeposition which provides a gentler treatment. In summary, CGS will not split water without an external bias due to the high flat band potentials. Also, a platinum treatment can be developed to increase the photocurrent produced by CGS. However, the standard platinum treatment is probably too detrimental to the film and so a gentler treatment should be used, such as a colloidal platinum treatment.

Stability of Light Harvesting Complex II (LHCII) in Synthetic Block Copolymers

Dmitriy Smolensky (TOWSON UNIVERSITY, TOWSON, MD 21252), Hugh M. O'Neill (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Alternate and renewable energy remain at the forefront of research. With the rising prices of fossil fuels and their political implications, new and improved methods of harvesting renewable energy are sought. One emerging field in research is creating biomimetic systems that mimic natural photosynthetic systems. The overall goal of the current research is to create a synthetic analogue of the supramolecular architecture of photosynthetic systems. As a first step we are investigating the properties of plant Light Harvesting Complex II (LHCII) and its interactions with synthetic membrane forming block copolymers. LHCII is a protein found in the thylakoid membrane; it is responsible for light harvesting and also regulates the rate of photosynthesis. Research to date investigated the interaction of LHCII and synthetic block copolymers, Plurionics®, which are tri-block copolymers consisting of two hydrophilic chains, polyethyleneoxide (PEO), and a central hydrophobic chain, polypropyleneoxide (PPO). The Plurionics® we examined were P123(PEO20 PPO70 PEO20), P105(PEO37 PPO56 PEO37), P84(PEO19 PPO43PEO19) and L62 (PEO6 PPO34 PEO6). LHCII was extracted from market purchased spinach by a series of steps including detergent solubilization, membrane aggregation and differential centrifugation. Circular dichroism (CD) spectroscopy was used to determine if the protein remained in its native conformation in the presence of block co-polymers. The protein-bound chlorophyll elicits a CD signal whereas free chlorophyll does not. In our studies, L62 stabilized LHCII compared to P84, P123 and P105. LHCII in 2.5% (w/v) L62 retained its chlorophyll CD signal for at least 24 hours. In conclusion, these experiments show a correlation between block-copolymers with shorter hydrophilic chains and stability of the LHC II complexes. In future work, these studies will be complemented with dynamic light scattering and small angle X-ray scattering to study the supramolecular structures of LHCII in block copolymer systems.

X-Ray Scattering Combined with Atomic Scattering Theory and Molecular Modeling to Correlate the Structures of Organometallic Molecules with Their Functionality

Allison Tovo-Dwyer (UNIVERSITY OF CHICAGO, CHICAGO, IL 60637), David M. Tiede (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). The recent energy crisis has caused people to look for new sources of energy. Solar energy is widely viewed as the most important, truly sustainable source of energy, although there are fundamental barriers preventing development of efficient solar technologies. For this reason, there is interest in understanding the fundamental solar energy conversion processes in nature and creating synthetic systems to duplicate them. When excited, certain organometallic compounds cause an electron to jump from the metal atom to an electron accepting molecule or an electrode, producing light-induced charge separation. Thus, these molecules are widely investigated as a basis for creating a photovoltaic cell, a device which converts solar energy to electricity. Until recently, most molecular structures have been determined in their crystal form. Even so, many molecules, including our molecules of interest, function in solution and each molecule's functionality is dependent not only on its structure but also on its environment. Thus, it has become necessary to study these molecular structures in solution in order to correlate function with structure. Ongoing research at the Advanced Photon Source is developing techniques for ultrafast measurement of X-ray spectroscopy and scattering for ground and

excited states of organometallic molecules in solution. The excited state data is collected by hitting the molecule with a laser immediately before probing the molecule with a 100 ps X-ray scattering pulse. Unfortunately, this scattering data alone is unable to provide the structures of the molecules in solution. Instead, we designed models of possible structures for the molecule and then, using scattering theory, calculated theoretical scattering patterns for these models. Finally, by comparing the theoretical scattering to the experimental scattering we were able to fine-tune our structural models as well as be able to test the reliability of these modeling programs. By gaining an idea of how the structure of these molecules in solution correlates with their function, we are able to move closer to developing a synthetic method of converting the sun's solar energy to electricity.

Core-Shell Structure of a-Manganese Dioxide Coated by Iron Phosphate

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Lithium-manganese oxides are attractive for use in lithium-ion batteries due to their safety, low cost and low toxicity. However, the dissolution of manganese (Mn_{3+}) into the electrolyte, side reactions between the electrode and electrolyte, and the formation of a solid electrolyte interphase (SEI) can limit performance of these materials. The aim of this study was to prepare a-manganese dioxide, (a- MnO_2) nanowires with electrochemical properties that overcame these problems through an iron-phosphate ($FePO_4$) coating. We developed a novel coating method that allowed uniform and controllable coating of iron phosphate on the surface of a- MnO_2 nanowires via an in-situ displacement redox reaction. We used Fe_{2+} as a reducing reagent for a- MnO_2 in the presence of phosphates. The thickness of the coating was controlled by varying the molar ratio of Fe_{2+} to MnO_2 . The a- MnO_2 dissolved completely in the presence of excess Fe_{2+} . We imaged the wires and the coatings using transmission electron microscopy (TEM); these images revealed that the wires had a uniform amorphous iron-phosphate coating. The TEM images also showed that the diameter of the MnO_2 core became smaller as the thickness of the $FePO_4$ coating increased. This observation was in agreement with the X-ray diffraction (XRD) data, which showed that the a- MnO_2 peaks became broader as the $FePO_4$ coat became thicker. TEM and XRD data were reconciled with a model in which a- MnO_2 dissolves through a redox reaction with concomitant growth of the iron-phosphate coating. Electrochemical testing of coated and non-coated nanowires did not provide evidence for improved performance of the $FePO_4$ -coated material, for samples heat-treated at 275 °C. Further electrochemical testing is now underway, for samples heat-treated at 400 °C. Heat treatment to this temperature should remove residual water and ammonia from the samples, which likely interfere with the performance of the material. We will continue to investigate the electrochemical performance of the $FePO_4$ -coated materials as a part of this study. Meanwhile, the use of different MnO_2 nanostructures in the coating process, or the full replacement of MnO_2 by $FePO_4$, may lead this study or other researchers to prepare other materials with enhanced electrochemical properties for lithium-ion batteries.

Detecting Trace Ambient Pesticides in Real Time Using Single Particle Aerosol Mass Spectrometry (SPAMS)

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Pesticides are widely used in both household and agricultural environments to keep homes and crops insect-free. Unfortunately, since even trace amounts of common pesticides can pose serious hazards to the environment, public health and homeland security, it is vital to carefully monitor pesticide usage. Past events, such as the deadly accumulation of the pesticide DDT in the food chain in the 1960s, as well as unforeseen future threats, which might exploit structural similarities between organophosphate pesticides and deadly neurotoxins, provide motivation for the development of a versatile method of detecting trace amounts of pesticides in real-time. This research demonstrated that Single Particle Aerosol Mass Spectrometry (SPAMS), a technique with existing applications in detecting biologics, pharmaceuticals and explosives, shows promise as a real-time pesticide detector. To test the SPAMS instrument's ability to identify aerosolized pesticides in heterogeneous media with high sensitivity, the instrument was used to obtain spectra of five common pesticides: malathion, dichlorvos, permethrin, carbaryl and imidacloprid. Compounds were aerosolized in either ethanol or water using a nebulizer, and the resulting aerosols were directed into the instrument for analysis. After correlating mass spectral peaks with likely molecular

fragments for all five compounds, this information was used to aid in the detection of permethrin and carbaryl in common household insecticides: Raid™ Ant spray and a flea collar. This research demonstrated that SPAMS can be used to detect pesticides in the ambient air, with no need for extensive sample preparation. Novel applications of SPAMS to situations requiring real-time, accurate pesticide detection were proposed.

Factors Affecting Signal Levels in HPTLC/DESI-MS of Dipeptides and Tryptic Peptides

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Desorption electrospray ionization mass spectrometry (DESI-MS) is a recently developed atmospheric pressure surface sampling/ionization technique that combines easy sample prepreparation and high throughput analysis with the high sensitivity and selectivity of mass spectrometry-based detection. Our group has been examining the use of DESI as a means to couple thin-layer chromatography (TLC) and MS. One focus has been the TLC separation and subsequent DESI-MS characterization of mixtures of peptides from a protein tryptic digestion. During these experiments, it was discovered that ionization efficiencies for peptides varied dramatically for a single protein digest, and that the nature of the separation phase and DESI spray solvent were important variables. To systematically examine the reasons for these observations, a series of leucine-containing dipeptides were spotted and digests of five common proteins were separated on different separation phases and analyzed using different DESI spray solvents. Dipeptide signal response was influenced by spray solvent and amino acid composition. In general, signal levels were higher when acetonitrile was used as a spray solvent than when water was used. The difference between signal levels using water and acetonitrile appeared to correlate with the calculated hydrophilicity of the dipeptides. More hydrophobic dipeptides gave a higher signal with acetonitrile as solvent, whereas more hydrophilic dipeptides gave a more intense signal when using water. There was a direct correlation between signal strength and hydrophilicity on a hydrophobic C18 reversed-phase TLC plate. With the protein digests, a trend was found between retention factor and peptide hydrophilicity values. However, the relationship between the two variables and signal response appeared to be more complex. These results suggest that spray solvent, stationary phase and amino acid composition are all important factors in DESI-MS signal intensity. Further study of the effects of spray solvent pH and the influence of capillary and plate temperature will improve the ability of DESI-MS to accurately characterize peptide mixtures.

Separation of Mixed Non-f Fission and Activation Products

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The separation of fission and activation products from nuclear materials for the purpose of quantitative analysis is a daunting task, but quite useful given its applications in national security and nuclear waste management. The project involved testing a proposed chemistry sequence for separating these products (representing 15 different non-f elements), which adjuncts to the actinide separation method currently in use. The chemistry is being tested by making elemental standards with known compositions of stable isotopes of the possible non-f fission and activation products. As great a degree as possible of separation for these products is desirable to avoid interference during measurement by gamma spectroscopy. A variety of separation methods were used including organic solvent extraction, carrier precipitation and ion exchange chromatography. Analysis was carried out with an Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES). The available test results suggest 80% conservation of elements through the separation process. The exception to this is Au, which appears at low concentrations, probably due to sorption on glass surfaces. A preliminary run through an anion exchange column was able to remedy this kink by removing the gold before it has the opportunity to cling to the glassware. One of the unpredicted effects of a 2-heptanone extraction targeted towards iron was the removal of Mo, Te and W. Whether this unintended separation is helpful or will have to be negotiated later on during the ion exchange chromatography is not yet known. Due to the usage of highly concentrated acids and HF as solvents in the anion exchange portion of the chemistry, extreme dilution of the eluate was necessary to eliminate interference and prevent damage to the ICP-OES. Unfortunately this resulted in such low concentrations of the elements of interest that it was pushing beyond the accurate detection limits of the ICP-OES and entering into the concentration range where environmental contamination can

significantly skew results. These effects made it impossible to gather any conclusive or truly informative data in the time period over which the experiment was run. While this chemistry is a worthy addition to the separations currently practiced, and generally produces good yields, further fine tuning and optimization is desirable to make the process faster and more efficient.

Ionic Liquids — New Materials for Green Chemistry (Part I: Making Ionic Liquids and Studying Their Properties; Part II: Recovering Cellulose from Filter Paper Using Ionic Liquids)

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The primary purpose for this project was to create a secondary-level educational module that introduced the students to ionic liquids (salts that melt below 100 °C) as possible alternatives to volatile organic compounds in industrial applications. Ionic liquids are unique organic salts with extremely low vapor pressure and the capability of dissolving a wide range of materials. Although the concept of ionic liquids has become well recognized among scientists, it is also important to educate a broader population. Up to now, the availability of pre-college level teaching materials on ionic liquids and green chemistry has been very limited. The uniqueness of this project lies in its role as one of the early attempts to ignite interest among secondary science educators and students about ionic liquids and green chemistry. The module consisted of materials and demonstrations for teachers, and two lab activities for students. The first lab activity involved synthesis of an ionic liquid based on a eutectic mixture: urea/choline chloride (molar ratio: 2:1) mixture, and an exploration of its properties by investigating the solubility of various species in the mixture. The results indicated that metal oxides (copper (II) oxide and iron (III) oxide), cellulose (filter paper), salt, sugar and artificial sweeteners had different levels of solubility in the mixture. The second lab activity applied the ionic liquid as extreme solvent for cellulosic materials. Ashless filter paper (No.41) was dissolved in the urea/choline chloride ionic liquid mixture (0.50% wt/wt). Then cellulose was successfully recovered from the ionic liquid solution. The design of the module carefully considered the pre-college students' chemistry background. After the module was modified to better suit the students' capacity at the suggestion of a high school student, it was field-tested in an "ionic liquids workshop" for the CSSP (Community Summer Science Program) students. From the students' pre and post assessments and classroom responses, it was clear that the module was relatively effective in educating secondary-level students about ionic liquids and green chemistry. The effectiveness of the module also helped to increase student interest in the possibility that such scientific research may lead to a more benign living environment.

Computer Science

Cellular Service Coverage Mapping Project

Paul Adams (MERCER UNIVERSITY, MACON, GA 31207), Don Williams (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Once a luxury, cell phones are quickly becoming a commodity taken for granted. As the information age booms many consider cellular technology essential for both staying up-to-date and working efficiently. Located on a federal reserve away from commercial areas, Oak Ridge National Lab (ORNL) suffers from poor cellular signal coverage, particularly in buildings. In order to remedy this problem and allow both employees and guest scientists to stay connected, the ORNL Information Technology (IT) division is taking steps to install signal boosting repeaters starting with a cellular signal survey of the major carriers. As the IT interns, my partner (Carolyn Shields) and I were provided with three cell phones each tied to a different cellular service network: AT&T, Verizon and Sprint. Using codes provided by the cell companies, we were able to enter an engineering mode on the phones that told us the dB signal strength each phone was receiving. We took floor plans of the occupied ORNL buildings and, using the provided phones, recorded the signal strength of each service provider at intervals through each building. The readings on the resulting maps were then highlighted to accent the difference between areas with strong existing signals versus dead areas with poor or negligible signal strengths. We found that the majority of ORNL buildings had mediocre to poor cellular coverage overall and areas with no coverage were much more prevalent than areas with strong signal strengths. We further noted that Verizon tended to have the strongest signal strengths and Sprint the weakest. However, while Sprint frequently had a weak signal, it had a persistent weak signal. AT&T, while tending to have a better signal strength, also appeared to require a stronger signal and would frequently have no available service. The surveys we completed will be used both to demonstrate the need for improved cellular service for

ORNL workers and to identify which buildings have the greatest need to have repeater systems installed. Funding is allocated piecemeal, so it is critical that the buildings which have the most to gain receive signal repeater systems first. Conducting signal surveys was a key step in the prioritization process.

Loadable Hypervisor Modules using the Xen Hypervisor

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Virtualization is an abstraction of hardware whereby the standard execution environment is isolated into a virtual machine (VM). The VM is managed by a virtual machine monitor (VMM), or hypervisor, which maintains the application binary interface (ABI). The use of a VMM can increase overall machine efficiency in terms of resource usage, enable customization of the execution environment for a particular application, and increase fault tolerance with the ability to migrate VMs. Because of these benefits, the area of High Performance Computing (HPC) has recently gained an interest in exploiting virtualization. The Xen hypervisor provides a reasonable basis for research into virtualization for HPC because it is open source and freely available. However, Xen currently lacks certain features that would be beneficial for research into an HPC VMM. For example, the ability to dynamically modify a kernel at runtime for debugging or performance reasons is beneficial and is done in other systems like Linux through loadable kernel modules (LKM) and kernel instrumentation probes (KProbes). Our work is employing a similar approach by adding loadable hypervisor modules (LHM) to Xen that can serve as the basis for an instrumentation system at the core hypervisor level. These new mechanisms will improve the runtime diagnostic and performance analysis capabilities of Xen and serve as the basis for future work in virtualization for HPC. Ultimately, the LHMs are used to extend the hypervisor allowing runtime operations like instrumentation, i.e., the modification of code currently in use at runtime. We are enhancing this VMM to support such runtime modifications. The development and testing involved the following: x86 and x86-64 machines with Intel VT-x virtualization extensions, the Xen 3.2.1 hypervisor and Linux 2.6.18.8 kernel, and Kernel-Based Virtual Machine (KVM). The modifications made to Xen and Linux created LHMs which are based on LKMs used by Linux. LHMs can then be loaded and unloaded to extend Xen and provide a basic mechanism needed for instrumentation of the hypervisor, for example, tracing annotations to assist in debugging or profiling of the hypervisor. As of this writing, LHMs may be loaded/unloaded to the Xen hypervisor. However, the ability to safely instrument the hypervisor is still under development. LHMs offer dynamic extensibility at the hypervisor level which allows for runtime modification without restarting the VMM.

Numerical Calculations for Ion Scattering in CARIBU

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The development of the Californium Rare Isotope Breeder Upgrade (CARIBU) for the Argonne Tandem Linear Accelerator System (ATLAS) facility at Argonne National Laboratory (ANL) necessitates computer simulations of ion behavior. A significant part of these simulations is the determination of the scattering angles of impinging ions upon He gas in a gas-cooling chamber. Because the numerical integrations required to calculate the exact scattering angle for ion-gas reactions are complicated and computationally intensive it is necessary to find a closed-form expression which gives values that approximate the results obtained from direct integration. Building upon earlier results obtained by Guy Savard for ^{133}Cs ions, we attempted to find an expression capable of accurately representing the scattering angles angles for non-Cs-He (i.e., in which the impinging ion is not ^{133}Cs) systems and for systems with laboratory frame energies up to 30 eV. Our results have shown that, while it is not difficult to extrapolate from earlier results to higher energies, mass dependence cannot be taken into account using curve fitting without considering the details of the interaction potential between the interacting atoms. The parameters necessary for performing such a fit are not available in the literature and, using the available data, we can only produce functions which mimic the general trend of results for mass-dependent scattering interactions. Our final equation, though complex, gives accurate results for ^{133}Cs in the region of interest and reasonable results for other systems. Future calculations of potential parameters based on ion drift measurements are necessary to determine the exact mass dependence in scattering interactions.

XOSCAR

Robert Babilon (SOUTH DAKOTA STATE UNIVERSITY, BROOKINGS, SD 57006), Geoffroy Vallee (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). The Open Source Cluster Application Resources (OSCAR), a software

suite for the deployment and management of high performance computing (HPC) clusters, currently provides two user interfaces: a command line interface and a graphical user interface (GUI). Since OSCAR aims to automatically provide the best HPC practices for the management of HPC clusters, it is crucial to provide suitable user interfaces that abstract problems for the management of distributed systems. Currently, this is even more crucial since cluster architectures may differ greatly among different HPC platforms. For instance, modern clusters are often composed of input/output, compute and login nodes, and sometimes virtual machines. Therefore, this research focuses on developing a modern GUI for OSCAR. The existing GUI was designed and built using first generation GUI tools, making it difficult to extend and maintain; this new GUI uses modern libraries and tools to expedite the support of new features and maintenance. The GUI, based on Qt-4.2 and C++, a programming language, can be developed on a standalone desktop without a cluster. Step one was to stabilize the initial prototype that only implemented the basic features. With a stable version of the basic GUI in place, it was possible to start designing and implementing new features such as virtualization, and system partitioning support. In order to improve the interaction with the OSCAR core, multi-threaded support has also been implemented in the GUI. The new thread management system of the GUI ensures that it remains responsive during extended runtime. In order to improve data persistence between the various GUI features, a system for temporal storage and user interaction has been implemented. The GUI will now warn the user prior to data loss and query them to select an appropriate action. The cluster network configuration feature has also been improved substantially by validating the user's input and improving the user interface. The new prototype GUI has progressed significantly since its inception. This development has brought the GUI to the next stage by preparing it for better thread management and tracking of modifications. The GUI is now able to handle more OSCAR core commands while maintaining thread synchronization. Future work will add more features such as removing/modifying cluster partitions, including the improvement and the addition of cluster software and network configuration capabilities.

Optimizing Inner Dot Product Kernels on x86 Processors

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Many scientific applications are dependent on a number of matrix-matrix and matrix-vector multiplications for performance. These operations, in turn, can be implemented using a few small, internal, dot product-like kernels. In this project, we show how to accelerate the single precision real versions of these kernels on modern AMD and Intel processors. The bulk of these codes execute efficiently, but some situations require that the four elements of an accumulating register all be added together and stored, a slow process called horizontal addition. We coded nine common dot product kernels with Intel assembly intrinsics and benchmarked them in blocked and unblocked matrix multiplications on both an AMD and an Intel processor to test the effects of different horizontal adders. We varied matrix dimensions to show how quickly each kernel reached its maximum performance while timing all functions with the Gnu C Compiler's OpenMP implementation. For both processors, a specialized kernel without a horizontal adder provided the best performance. For the cases that required the horizontal adder, specific situations dictated the winner. Testing also revealed certain instructional weaknesses on both processors. This information can be found in manufacturer documentation, but it is rarely comprehensive. Further, it is difficult to predict how modern out-of-order, super-scalar architectures will behave on real code. This work provides empirical, instruction-level information for programmers seeking the highest level of performance in their dot product and matrix operations.

Development of Data Collection and Display Programs for the Collider-Accelerator Controls Group

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The Collider-Accelerator Department (C-AD) Controls group at Brookhaven National Laboratory (BNL) constantly works to improve the software used in data collection and management in order to make analyzing the particle accelerators' data easier for the scientists working at the lab. To this end, three software programs were developed for use by C-AD. These programs were written in C++ and rely on C++ libraries and classes available at BNL, including the XMLDom library, the dbtools library and the UI library. A program called "WhatsBeingLogged" was used in order to gather information about which data has ever been logged at the lab. The first program written was used to determine the logistics of switching over to a data-logging

model for the collider-accelerator complexes where all existing data is logged. Currently, only data asked for by users ahead of time is logged. The program looked through what was currently being logged during runs and determined that that approximately 15% of all properties were currently being logged, meaning that about seven times more disc space would be needed to log all available data. These results were close to what was expected, and show that switching over to the proposed model would not be extremely cost-prohibitive. A second project was to improve printer administration and graphical user interfaces (GUI). In order to make the process more intuitive, a database infrastructure in the form of XML files was created to store the list and descriptions of available printers. User interface tools were then developed to make for easier, more intuitive selection of printers than the current system in place provided. The final program developed was used to gauge the accuracy of the ntpserver, which keeps the times of all the C-AD computers in sync with one another. This program was run every ten minutes for two weeks, and compared the times on ten computers within the network. During this period, there was never a point at which the time could be verified to be more than one second off between the computers, meaning that the ntpserver is working to keep accurate time between the department's machines. With these improvements, particularly the new printer GUI, it has become much easier for those working in C-AD to go about their day-to-day work.

Automated Inventory with IRobot Create and Radio-Frequency Identification

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The goal of this project is to use robotics and radio frequency identification (RFID) equipment to enable automatic inventory checks in an office setting. Roomba is a robotic vacuum cleaner manufactured by iRobot. The disc-shaped robot uses simple wall-following, spiral and angle-changing algorithms that will theoretically cover and vacuum any size room. The Create, also made by iRobot, is a Roomba-sized robot without the vacuum, which is explicitly designed for robot development. The Create is programmable in C code, allowing for the programmer to read the values of the various sensors on the robot as well as to control its movement, lights and sounds. Using this technology, the Create will be programmed to periodically navigate around an office building, holding an RFID (Radio-frequency identification) tag reader that will take inventory of tagged items within the building. Once it has completed its scheduled inventory check it will return to its base unit to charge its battery and await the next scheduled check. This summer, the focus was on the navigation and scheduling of the Create robot.

Fabrication Laboratory

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Fab Lab is an abbreviation for Fabrication Laboratory. It is a group of off-the-shelf, industrial grade fabrication and electronic tools with open source software to create product prototypes. This software can read the different kinds of ways in which people describe things digitally and turn them into tool paths for all of the different ways it's possible to make them. Setting up Fab Lab is a complex interdisciplinary project which involves equipment and supplies procurement, facilities and environmental setup, software installation, network setup, hardware interconnections and training for support and end users. Although there are several Fab Labs already deployed around the world (there is one in Chicago's Museum of Science and Industry), there is hardly any documentation available about installation procedures and system setup. The information is mostly limited to an equipment inventory, and the user's information is just as scarce. In order to bring the Fab Lab to Argonne we are using the Fab Lab at the Museum of Science and Industry as an example to follow. The initial research of the existing facilities has been completed and all the information gathered to setup a Fab Lab at Argonne. The next step is the documentation of the use of its equipment and its capabilities. The goal at Argonne is to create a Fab Lab cookbook that will record a step by step procedure of how to do projects with Fab Lab, including the equipment needed, skills required and estimated time to complete each project.

Implementation of Automatic Differentiation Tools in the Network Enabled Optimization System Solvers

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Although a number of solvers implemented in the Network Enabled Optimization System (NEOS) Server can use derivative information provided by Automatic Differentiation (AD) tools, only a few of the available AD tools are implemented in any of these solvers. The objectives of this project were to: (1) implement these AD tools in the NEOS solvers, which could use AD for derivative computation; (2)

develop a method for re-executing jobs submitted to the main server by using all AD tools for the respective programming language; (3) set up regression testing to identify problems in specific AD tools; and (4) connect NEOS to AD tool installations that can be easily updated to their latest releases. A number of old Perl scripts enabling the compilation and execution of the Open AD tool were updated and rewritten into Python, simplifying the implementation of Open AD in NEOS. Subsequently, by using Python scripts in conjunction with solver and tool-specific makefiles, a new infrastructure was created for the implementation of AD tools in NEOS solvers. The AD tools Adic, AdolC, Adifor and Open AD have been implemented in the NMTR and BLMVM solvers, while Adifor was re-implemented in the TRON solver. A method was developed for executing NEOS submissions off-line by using all other AD tools for the given programming language of the submission. This approach permits both regression testing and solver robustness if the primary AD tool should fail. The abstraction of the AD step from job parsing and execution and the homogenization of AD tool implementations allow the solvers to use an identical execution protocol with all implemented tools and allow generalization of the AD step for all solvers. Thus, simple updating of tool releases is possible, as is the implementation of new tools within the solver, and AD tools already implemented in other AD-compatible solvers has been facilitated.

Electronic Conversion of the Training Action Tracking System for the High Flux Isotope Reactor

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The High Flux Isotope Reactor (HFIR) is one of only two Category-A nuclear facilities managed by the Department of Energy (DOE). HFIR-specific training programs are required to be in strict adherence with DOE-5480.20A "Personnel Selection, Qualification and Training Requirements for DOE Nuclear Facilities." The project focused on transforming the paper process of altering training material at the HFIR into a completely electronic process. The goal of the Training Action Tracking System (TATS) is to ensure that the training program is relevant and up to date with current HFIR plant configuration. Any time a drawing is changed, specification is altered, or modification is made, there could be an impact on how workers are trained. Last year there were almost nine hundred of these changes which resulted in two hundred and twenty-five training staff hours spent on wasted routing time. Adobe ColdFusion 8 and JavaScript were used to write a web browser application. The application utilizes several methodologies within software programming, such as Model-View-Controller, Object-Oriented Programming, Factory Method and the ColdFusion specific methodology FuseBox. Database interaction was conducted in Structure Query Language and then utilized by ColdFusion. The system seamlessly integrates with current HFIR web-based systems that are used to address plant modifications, plant maintenance, plant procedures and plant safety analysis. When an item is completed in the aforementioned systems, the TATS application generates an item and alerts the training staff via email that there is a new action item for review. Training staff now has the opportunity to decide if a change in the training process is required. The application substitutes an average of three clicks in place of a signature, date and the transportation of paper from one location to another. No longer is it necessary to print, file, or maintain records; training staff now only needs to review the items under consideration. The HFIR Training Officer, who formerly coordinated the entire route, is completely removed from the process, improving efficiencies. In addition, conversion from human data entry to automated data entry significantly reduces the potential for human error. The difference in time spent by using the application instead of the old manual method will save the Research Reactors Division around \$1500 per month in wages and overhead.

Characterizing the Input/Output Behavior of Parallel Applications

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The purpose of this project is to characterize the input/output (I/O) behavior of parallel applications and benchmarks. By better understanding how the I/O operations behave in parallel applications, we will be better equipped to understand and predict how I/O will behave on future systems, even before they are created. By predicting how the I/O will behave, we can estimate what kind of system will be the most efficient to build and run a certain application, and at what scale that application will be able to run on that machine. To observe the I/O behavior of the parallel programs, we used VampirTrace (VT) and Open Trace Format (OTF) to trace benchmarks and applications running on a Linux cluster using parallel file systems such as PVFS and pNFS. Our goal was to get answers to questions such as: What I/O functions are being called? When are they being called? How often are

they being called? What function are they being called from? To answer these questions we used the output from OTF and VT to look closely at the applications I/O behavior. We developed two tools to scan the OTF files generated by VT; these tools organize and present this information in a way that characterizes it clearly. The first tool calculates which node is using the most time to complete its I/O functions. It also finds the minimum time, average time and the standard deviation for each I/O function. The second tool calculates the maximum, minimum and average file operation sizes of Portable Operating System Interface functions called by Message Passing Interface I/O (MPI-IO) read and write functions along with the standard deviation and the combined total of these values. This tool showed that there are small 24 byte reads being performed inside of a benchmark function testing parallel write performance. This was unexpected, because it is a high-level write function and we had expected such functions to make calls to write functions only. The information we have gathered from these tools will be useful going forward; they have already helped us detect some unexpected behavior in a MPI-IO benchmark. They also can give developers, users and systems designers additional insight into how the high-level functions are handling the I/O for their programs.

Exploring Multi-Core Limitations through Comparison of Contemporary Systems

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The objective of this study was to evaluate the performance of contemporary multi-core platforms, AMD Barcelona and Intel Woodcrest, for scientific applications. Analyzing the performance of these systems allows us to identify system parameters and configurations that could yield optimal performance for data and compute-intensive scientific kernels. Since these multi-core processing devices are building blocks of the world's fastest supercomputing systems, the insights into performance behavior not only enable us to optimize large-scale scientific simulations but also provide guidance for designing future high performance computing resources. I ran the High Performance Computing Challenge (HPC) benchmarks on the target systems to compare the Linpack (HPL) and Double-Precision General Matrix Multiply (DGEMM) results. HPC benchmark suite represents workload behavior of a wide range of scientific calculations. HPL in particular is used to measure performance of the world's fastest supercomputing systems. I used two performance tools, the GNU profiler (gprof) and Tuning and Analysis Utilities (TAU), to understand the workload characteristics and to closely examine the performance behavior with call graphs and flat profiles on the targeted platforms. The HPC benchmarks performed within the expected range on the Intel Woodcrest, but delivered a large discrepancy in results on the AMD Barcelona platform. The DGEMM results were within the expected range of a high percentage of the theoretical peak for the Barcelona system. However, the HPL results were consistently a third of the expected Floating Point Operations per Second (FLOP/s) value. I examined the function call graphs to determine which sections of the HPL code were causing the slowdown, and I discovered several functions that consume 40–50% of the lost time. The main culprit, the function HPL_lmul, is a series of arithmetic operations done via bit shifts in register. The HPL results on the Intel Woodcrest platform demonstrate that multi-core benefits compute-intensive applications because efficiency per socket is high. The results on the AMD Barcelona, however, drive home the point that without a multi-core aware optimization, mapping and placement schemes, the performance will deteriorate as the number of cores per socket increases thereby increasing resource contention such as memory bandwidth among cores within a socket.

Providing a Foundation for the Analysis of Large Data Sets and a Framework for Network Analysis

Jon Dobson (EAST TENNESSEE STATE UNIVERSITY, JOHNSON CITY, TN 37614), Line Pouchard (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). In parallel computing, many tasks can be performed simultaneously. However, performance factors such as communication, synchronization and computation can negatively impact the performance of parallel machines. Current methods for locating bottlenecks and points of failure on parallel machines can generate a tremendous amount of data. The objective of the Oak Ridge Computing Analysis Tool (ORCAT) is to provide a foundation for the analysis of large data sets and a framework for network analysis. ORCAT is implemented in C++ and utilizes a number of open source libraries. Developing a serial prototype was useful to better understand the requirements of a parallel application and to build a tool that will receive millions of input streams for relevant analysis. Pattern Language for Parallel Programming (PLPP) was used to identify the requirements of running the application in a High

Performance Computing (HPC) environment. The result of this work is a flexible software tool that can be used to download, tag, analyze and search text or sensor data. Prototyping the ORCAT framework with text data allowed rapid testing without obtaining actual sensor data. Further work will allow ORCAT to monitor and analyze thousands of sensors in a HPC environment.

NetPIPE: Network Protocol Independent Performance Evaluator Version 5.0

Torrey Dupras (NORTHERN MICHIGAN UNIVERSITY, MARQUETTE, MI 49855), Troy Benjegerdes (AMES LABORATORY, AMES, IA 50011).

Ames Lab's Scalable Computing Lab (SCL) created NetPIPE as a conceptually simple performance benchmark used to visually represent the bandwidth latency trade offs of high performance computer networks. The simple design allows for a single benchmark code to evaluate multiple protocols, such as ethernet, InfiniBand and Myrinet as well as multiple Application Programming Interface (API) layers, such as Message Passing Interface (MPI), Transmission Control Protocol (TCP) and shared memory. To extend and enhance NetPIPE's capabilities, the SCL is developing a third generation version to allow for more sophisticated user interface as well as provide rapid application development and an object-oriented design. The Python programming language has been chosen for its object-oriented nature, ability to link to the existing NetPIPE C code modules, and to leverage open source analysis and visualization frameworks, such as Pylab, Numpy and MayaVI. The SCL used the Pylab tools to analyze a 1000 benchmark runs of the original NetPIPE 3 and the new NetPIPE 5 code. Analysis showed good statistical correlation using linear regression methods and visual representations. Further research and analysis is needed to identify the cause of anomalies discovered in the results.

* Design and Development of Wireless Applications for Midwest Center for Structural Genomics

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The Midwest Center for Structural Genomics (MCSG) at Argonne National Laboratory is used to develop and optimize integrated methods for the determination of protein structures through X-ray crystallography. The goal of this project is to design and develop a smart client application to view existing protocols for high-throughput protein purification on the Pocket-PC screen and to develop a mobile Personal Digital Assistant (PDA) application with MCSG cloning and purification databases. The major areas of work during this project were to design and implement rich mobile web content and applications across a variety of hardware platforms and handheld devices. The PDA will exhibit the same functionality as a web page, but it will be much more convenient and accurate on a secure network. Current web applications were designed, implemented and upgraded for common web tasks and data storage to fit into the scale of a mobile window by using the most up-to-date technologies. The initial purification mobile applications were developed by using Microsoft.NET 2003. It will be migrated by using Microsoft.NET 2008 technology. User interfaces were developed with ASP.NET Mobile forms, HTML, and WML with C# programming and Oracle PL/SQL language. The mobile application will increase the efficiency of the data collection and analysis and minimize the errors that can occur when data are transposed from paper to computer. Users can scan the data by using an instrument scanner and save the data directly into the database. When users enter data in the mobile device, it will prevent them from entering invalid and out-of-range data by using validation controller. The mobile applications are able to deliver access to anyone authorized anytime, anywhere on any handheld device. With this greater convenience and security, scientists will be able to continue their research in the laboratory as they implement their data.

Implementation of Change Management

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No central, automated system previously existed for approving changes within the Computing and Information Sciences division. Such a system was developed this summer using the Numara FootPrints software, a service desk management solution used to implement a ticket submission and approval process. Implementation took place in two phases. The first involved designing the user interface, what an employee sees after logging on to the FootPrints site to create a Request for Change (RFC). The appearance of this page was determined by creating fields prompting the user to provide information about the RFC. It was necessary to obtain extensive input from division employees, resulting in several iterations in making adjustments to the information fields. The second phase involved designing the workflow.

The Change Management module of FootPrints allows for the creation of approval processes the RFC must travel through. A process was developed for each of three categories of RFCs: standard, recurring and urgent. The processes include approval by a Change Approval Board (CAB) comprised of individuals representing major areas of the division and by one or more Change Managers. An automated system provides a faster means of approval, and a voting mechanism within this system allows for consideration of all aspects of each change, helping to avoid unforeseen problems. Becoming familiar with FootPrints was an important step in the project, but not as important as keeping the original goal in mind: creating a system that is easier, faster and more convenient to use than previous methods of change approval. Numerous benefits will be enjoyed by the division: an automated system will allow for a much quicker turn-around time, a centralized database will reduce confusion and increase organization, and a voting process in which many individuals voice their input will help avoid unforeseen problems.

GridFTP over Infiniband Technologies: Evaluation, Design and Implementation

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Data movement across distributed sites holds an ever greater stake in technology infrastructure, and therefore attracts a large amount of scientific interest. Although InfiniBand (IB) has been a cutting-edge interconnect for performance computing, the research community has not seen a complete solution for IB-based data movement in wide-area environments. Current data movement protocols (BBP, GridFTP, etc) utilize Transmission Control Protocol (TCP), potentially creating a bottleneck via use of IP over IB (IPoIB). In this research, we propose to provide a design and implementation of the GridFTP protocol on top of IB, taking advantage of its Remote Direct Memory Access (RDMA) mechanism for data movement. In conjunction, we will conduct an evaluation of GridFTP, comparing its performance on top several network mechanisms including IPoIB, Sockets Direct Protocol (SDP) and RDMA using our implementation of GridFTP over IB RDMA to address the goals of this research, we present the following studies. First, we install and investigate the basic performance of GridFTP on top of Gigabit Ethernet. Second, we explore GridFTP performance over an IB network via IPoIB and SDP. Third, we develop an implementation of GridFTP over RDMA, in which we introduce an RDMA-based connection management protocol and an RDMA-based extensible Input/Output protocol (XIO) driver into GridFTP. Finally, we compare the performance of this new RDMA-aware GridFTP to TCP, IPoIB and SDP-based file transfers. At this point in time, the first two studies presented above are complete. The data show that GridFTP file transfers over IPoIB or SDP outperform Gigabit Ethernet by 20–25%. This performance benefit was relatively constant across all transfer block sizes from 1 Kb to 1 Mb. Furthermore, no differences in transfer latency were observed between IPoIB and SDP. Baseline network performance data support these findings by noting a significant latency difference between IB and Gigabit Ethernet transmissions. However, baseline data does indicate a performance gap between IPoIB and SDP, a trend not observed in the GridFTP transfers. In conclusion, GridFTP over IB clearly outperformed Gigabit Ethernet within the parameters of the study. An RDMA-aware implementation of GridFTP is under active development, and may provide further performance benefit by bypassing the possible overhead of TCP. Further work will explore GridFTP performance in a WAN environment via the Open Science Grid.

Control Charts

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The Planning and Assessment team has a broad range of data on different assessments made around the lab but wants to begin spending more time analyzing the data collected. The team wants the data analyzed using statistical process control charts that tracks the data and shows if any trends are occurring. The team has used control charts in many of their other analyses but has not with these assessments. Before I could generate the control charts, I had to learn how to construct them. I studied many PowerPoint presentations and attended some instructional sessions on how to create control charts. Once I became educated on the development of control charts, I took the team's data from the Assessment Tracking System (ATS) and produced the necessary control charts. For the majority of the charts, trends were readily visible, but occasionally you would come across data that was disassociated. When this occurs, more data will be required to see if the numbers start to level off. By utilizing these control charts, the

team can now look at the past trends that occurred and make accurate predictions for future assessments. This will allow the team to make early actions to correct and improve what was being assessed. The only additional work the team will have to do will be to keep the control charts up to date. These control charts will help the company save time, money and resources by reducing the number of unexpected results identified in assessments.

The Impact of Different System-level Virtualization Solutions on High-Performance Computing Applications

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System-level virtualization is now widely used for server consolidation, i.e., the maximization of resource utilization executing virtual machines (VM) on top of bare hardware. Virtualization is of clear interest for high performance computing (HPC), isolating the application from the hardware and enabling fine grain resource management (using capabilities such as VM migration). The objective of this project is to evaluate the impact of different system-level virtualization solutions on HPC applications. Such evaluation implies two challenges: the configuration of a testbed and the execution of benchmarks for the evaluation of the overhead generated by the selected system-level virtualization solutions. Virtualization technologies are typically based on three different software operating systems (OS) (compared to the single software component on standard systems): (i) the host OS, giving access to the physical hardware, (ii) the virtual machines and (iii) the virtual machine monitor (VMM) which is in charge of exposing virtual hardware to VMs. Since our goal is to study the overhead generated by different system-level virtualization solutions (e.g., Xen), a method for the installation and configuration of those solutions is needed. This guarantees similar system environments for evaluation and comparison. Evaluation reproducibility is actually an important aspect of benchmarking. For that, we used research prototypes for the management of VMs, i.e., OSCAR-V and more specifically V2M. Our testbed is composed of an Intel dual-core machine and two Intel Xeon dual-core machines. The same OS is used for both the physical and virtual machines (Ubuntu-8.04 x86_64 server), and we execute the HPL benchmark. HPL makes use of a linear algebra library and is used for the Top500 list (the list of the most powerful HPC systems world wide). The selected virtualization solutions are KVM, QEMU and Xen. The first contribution of the study is the development of a method for a reproducible testbed configuration, a critical point for benchmarking. The next contribution of this study is the discoveries made while running HPL on the selected virtual machines. After running HPL on the native hardware, QEMU, KVM and Xen, it was found that the native hardware outperformed these virtual machines due to an enormous amount of overhead. Therefore, in order to use these virtual machines for HPC applications, an enormous amount of tuning must take place.

Development of a Tool Using MATLAB to Study Phase Drifts in the SLAC Linac

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The Main Drive Line (MDL) and L2 Reference Line (L2) at the SLAC National Accelerator Laboratory are used in timing the klystrons which power the accelerator structure. Archiver and Stanford Linear Collider (SLC) Buffer data was taken for the MDL and L2 and converted into data which could be easily handled by MATLAB. This data was recorded from the phase monitors located from sectors 21 to 30 for approximately one month and data points taken while the Linac (Linear Accelerator) was turned off were removed. The data consisted of the phase difference between the previous and next sector, and the temperature at the location this difference was measured at. This data was used to find correlations between the phase drift and temperature, and plots of their relationship were drawn as well. The data recorded showed that the MDL and L2 were experiencing approximately the same phase drift in their signals from sectors 21 to 24, to within 0.03 degrees S-Band (2856MHz) per degree Celsius. The phase monitors in sectors 29 and 30 were also found to have a weak linear correlation between the phase drift and temperature data. This data suggests that the thermal expansion joint system used in the MDL and the Helix used in the L2 reduce phase drift equivalently and the two lines could be used interchangeably with little to no problem. Sectors 29 and 30 should also be studied further; the feedback in sectors 27 and 28 may be causing irregularities in the data recorded from these sectors. Preliminary data was taken of the phase cavities in the Linac, which are used to directly compare the timing signal against the electron bunch. This data showed these devices to be precisely in phase and working properly.

*** Executing Code in Higher Security Context without Requiring a RunAs Password**

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The Windows security model for Windows XP provides for two basic users, Administrators and Limited Users. As a member of the Limited Users group, a user has certain limitations imposed, usually for security reasons. At the Accelerator Test Facility, the Pyrocam III camera is used to perform laser beam profiling on the CO₂ laser system. Currently, there is an issue with the Pyrocam III Camera (exact cause unknown) which causes the device to uninstall itself whenever it is powered off or disconnected. The infrared camera viewer then becomes unusable until the driver is fixed. Since the operator of the camera has not been granted administrative privileges, reinstallation of the device driver requires a second user with those privileges. Although granting the user the privileges would work, the ideal solution would be one that fixes the Pyrocam issues without changing those security settings. There is a program, sudowin, which can be used to elevate the privileges of the user, but it is not a stand alone solution and requires Microsoft's dot net framework. A program was created to facilitate the operator's need for reinstalling the Pyrocam driver without directly elevating his/her privileges. Programming development was done in C++, using Borland's Turbo C++ IDE. The Win32 API provided the necessary functions to search for and install the driver and Borland's Visual Component Library provided the tools to create a system service and also to create a graphical user interface. The solution consisted of creating two separate programs, each running in a different security context (one as Local System, the other as operator) and the use of Named Pipes to communicate between them. The solution is guaranteed to work under the condition that only one user is logged on. If more than one user is logged on, then the confirmation prompt for installing an Unsigned Driver may appear on any of the logged in user's screens. This solution allows the operator to continue using their Limited Account while still enabling them to install the driver for the Pyrocam device. Also by using the Local System account, we can also avoid having the users type in passwords to run the driver installation itself.

Software Tracking on the NCCS Supercomputers

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To best maintain the supercomputers managed by the National Center for Computational Sciences (NCCS) and provide the research scientists at Oak Ridge National Laboratory with the proper software to perform complex calculations and simulations, the NCCS staff needs to know which software is being used the most so stable upgrades can be applied frequently and which software is being used rarely, or not at all, so that time is not wasted by over-maintaining these libraries. In order to quantify and qualify this data, a method that stores what packages linked to an executable at link time and retrieves information about the executor at run time must be devised. These intercepts cannot affect the user's experience in any way, be it wasted time, failed builds, crashed runs, etc. To meet this objective, I researched the structure of an ELF executable and studied Cray Inc's model for automatically instrumenting executables. I found that various types of data and information could be stored in the section headers of ELF executables. Furthermore, portable assembly code can be written which will create a section header in an ELF executable. These section headers provide the logical place to store information about what libraries were used when the program was compiled. To retrieve and store this data, I wrote wrappers for ld (the linker) and aprun, Cray's job launcher for parallel codes. These wrappers intercept the calls to the executable versions of ld and aprun, respectively. The ld wrapper calls a C-executable that determines the full paths to the libraries specified on the link line and inserts this link line into a MySQL table. An object file containing instructions to add a section header named ".nccs", which contains the unique integer that references the table, is then added to the link line, which is then passed on to the real ld. The program is then linked to all of the libraries and object files found on the original link line along with the object file I created. The aprun wrapper calls a C-executable, which searches for the unique identifier in the section header of the user's executable and updates its own MySQL table with information that links it to the ld table. The real aprun is then called and the user's job is run. This method of tracking software has been put into production and we can now begin improving the efficiency of support offered to our users by generating usage reports based on the data we have and will collect.

Differential Algebra Module of the Unified Accelerator Libraries

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The Unified Accelerator Libraries (UAL) represent an open object-oriented software environment that integrates the broad range of accelerator codes necessary for simulating complex scenarios. This project specifically addresses the Differential Algebra (DA) package of the UAL. DA is one of the most important techniques used in computational accelerator physics. It provides a consistent set of operations on truncated power series and allows one to generate Taylor maps for various complex optical elements, such as the helical dipole of the Relativistic Heavy Ion Collider (RHIC), the wiggler used in synchrotron light sources, and the combined function magnet used in the deuteron Electric Dipole Moment (dEDM) project. In the previous version of the DA module, this approach was implemented in the Perl programming language with an eXternal Subroutine (XS) interface to call C++ methods. The Perl interpreter aimed to preserve flexibility and extensibility of UAL in the user interface layer. However, the use of two programming languages, C++ and Perl, introduced serious obstacles in debugging and maintenance of these complex applications. This project consolidates and enhances the previous applications in a new C++ based DA module. This module, with its new application programming interface, eliminates the need for an XS interface and creates a consistent framework for the new DA-based extensions. Furthermore, it facilitates the application of the DA approach in neighboring scientific domains by integrating with the corresponding C++ toolkits such as the ROOT data analysis framework and others.

Secure Data Dissemination: An Implementation of an Internal Search Engine Configured to Maintain Security and Efficiency

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One of the greatest benefits of the computer age is the ease with which large amounts of data can be transmitted over long distances and to large groups of people. However, within the setting of a national laboratory, data distribution must be handled with care, only disseminating the necessary information to the appropriate people, so as to maintain both crucial security and the laboratory's proprietary interest in the data. The focus of my project was the safe propagation of data through a variety of interfaces on the intranet of Lawrence Livermore National Laboratory (LLNL), with a special focus on internal searches. Much of this work is essentially the same as that done in the private sector. Freeware like ht://DIG, public domain source code from Google and Yahoo and experienced programmers are useful in planning the appropriate programming strategy. Yet the algorithms used must be configured in such a way as to be easily traceable by organizational administrators and to allow for validation of a user's identity. Further, for the continued success of any implementation strategy, an individual page needs to be easily removable from the database compiled by the crawling search engine, so as to not provide any chance of releasing restricted information to uncleared individuals as page content changes. The Google Search Appliance (GSA), configured for internal use and backed with LLNL's standard security parameters, was the most efficient implementation. Accomplished by the addition of ten lines of code added to a page's source, this technology would be easily scaled for further use in the Laboratory's various organizations. Also, this approach allows for the customization of output through various methods. For security reasons the customization method chosen here was direct manipulation of the GSA's returned Extensible Markup Language, parsing the results using JavaScript into a table included in the site's style sheets. This implementation provides results which are easily controllable by internal review to maintain security, but also provides results with the speed and accuracy of a professional search engine.

Transitioning from an ASP.NET Web Application to a SharePoint Web Part

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Software applications have a limited life span. Eventually the code or hardware becomes obsolete necessitating either discarding the existing application and starting over, or attempting to translate as much as possible into a new system that again meets the necessary specifications. The Tritium Technology Program (TTP) at Pacific Northwest National Laboratory was using one such application to rapidly find project reports. It still worked, but its implementation was less efficient than it could have been with newer technology and so was deemed worthy of an update. TTP staff was already using Microsoft SharePoint (SP), a platform with tools for content management and team collaboration, in its day-to-day operations so it was identified as

the host technology for the rebuilt application. The original application was programmed using ASP and ASP.NET which is theoretically compatible with SP, but the code needed to be simplified. Three steps were taken to replace the existing system. First, the model representing data stored in an SQL database was replicated using a List and a Document Library within SP. Next, a workflow was written to automate the process of collecting and storing metadata located in the report file names. Finally, a web part was built to replicate the user interface of the previous reporting application. As an added feature, the web part was built to employ the use of Asynchronous JavaScript and XML technology. The resulting SP functionality closely resembles the original application. Now all of the TTP applications are located on a single system and require less human interaction, thereby freeing both computing and employee resources for other tasks. In the future it will be easier to maintain a single SP environment with this added functionality than it was to maintain an SP server, an SQL server and a web server simultaneously.

Content Addressable Networks for Fault-tolerant Supercomputing
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In recent years the number of nodes present in high-end supercomputers has dramatically increased. Hence, the assumption that no node participating in a scientific application will fail during a single execution can no longer be expected to hold. A method for coping with node failures, which preferably does not require significant alterations to the code of parallel programs, is necessary. Methods have already been devised for providing a fault-tolerant, distributed infrastructure. Peer-to-peer networks, for example, commonly use distributed hash tables (DHTs) to store their metadata. This project explores the ways in which one type of DHT, a "content-addressable network" (CAN), allows a supercomputer to sustain node failures and transparently continue computing. The CAN algorithm is implemented atop the Message Passing Interface (MPI) instead of a traditional Internet-based protocol. Because MPI is portable across different supercomputer architectures, this makes software which uses it applicable to a wider variety of environments. Current implementations of MPI are, unfortunately, found to be unable to provide failure-handling behavior adequate for this application, but efforts are made to simulate its performance were such an implementation to exist. This allows it to become portable across different computer architectures. Several other adaptations are also made to better suit the requirements of high-performance computing.

Performance Tuning Utilizing Instruction Scheduling and Empirical Search

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The final goal of this project is to create an automated framework utilizing loop optimizations and real performance data to optimize general codes. The target program heavily utilized matrix multiplication, so work began on that subproblem. The first step was to look at other tools (ATLAS, ACML), which performed at 90% of peak, but gave very low performance on small matrices. That could either be due to large matrix optimizations not working well for small matrices, the programmers not being concerned with small matrices, or simply overhead due to function calling. Some of the good performers on small matrices made assumptions about the structure of the matrix which wouldn't be acceptable for a general purpose matrix multiplier. Toward that end, work was done on instruction scheduling and memory hierarchy issues, using a 4x4 matrix multiply kernel and expanding to a large matrix multiply kernel. It was quickly improved by using Single Instruction Multiple Data instructions instead of single operation instructions and eliminating the internal loops for ease of scheduling and performance. That removed the need to test loop transformations and memory hierarchy issues for the small kernel, so instruction scheduling was the next logical step. First was manual scheduling on the C source code and then scheduling the raw assembly code for more power, both by hand and then by a search script which attempted to model the actual CPU. Once the small one was sufficiently optimized, it was used as part of a large matrix multiplier. Future work will be on an overall framework for automated optimization of general codes.

*** A Computational Process to Locate Insertion Sequence Elements and Study Horizontal Gene Transfer in Bacterial Genomes**

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Currently, there is a tremendous focus on studying how whole units of DNA are shared between species. These movable tracks of DNA, called transposons, are demarcated by shorter insertion sequence (IS) elements, which themselves are generally around 700 to 2500 bp

in length and contain code for proteins implicated in the transposition activity called transposase. IS elements are bracketed by pairs of inverted repeats of variant length (approx. 10–30 bp) and are further embedded in a pair of short direct repeats of approximately 3–7 bp. While there is a great deal of software to automatically annotate genes and regulatory regions, there is currently only one known program to identify IS elements de novo. That hundreds of completed bacterial genomes are currently available and more are constantly being added to that list makes it increasingly important for the computational detection of IS elements. To this end, we have developed a program written in Java to locate IS elements in bacterial genomes. The process consists of two major components. The first identifies all inverted repeats within a given genome. The second searches the interiors of the candidate pairs for homology with transposase genes. In order to identify the inverted repeat sequences, the program first allocates storage space, then scans through the given sequence, recording the positions at which each possible 5mer is located. This data is then stored into a two-dimensional array which is then sorted through for printing. Preliminary tests of this process on the genome of *Enterobacter* strain 638, recently sequenced as part of the DOE biofuels initiative, revealed 9 putative IS candidates, 6 of which were confirmed by Blastx searches of Genbank, which yielded strong homology matches to transposase and integrase in other organisms. However, the inverted repeat sequences reported by the program did not, in most cases, match with those from annotation databases. Further testing on another IS-rich genome, *Cupriavidus metallidurans* (CH34), will allow us to optimize program parameters to improve performance. Because this process reports direct and inverted sequence pairs, which travel along with the IS element as it moves, it can be used to trace horizontal gene transfer history within or between genomes for evolutionary studies. These tests are part of an ongoing study and will be completed in the near future.

Improving De-Cloning Algorithms for Jefferson Lab's Hall A BigBite Spectrometer

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In particle physics experiments, the main method of determining the track of detected particles is through algorithmic computer analysis. As part of these algorithms' function, it may be necessary to perform de-cloning to collate multiple cloned tracks caused by a particle into a single entity, while also eliminating spurious detections. Generally, de-cloning can be handled by clustering algorithms, but good clustering algorithms are difficult to implement because acceptable run time and result stability are often at odds. The goal of this research was to overcome these limitations by developing an algorithm with a fast run time but a consistent and high tracking efficiency and study it for use in multi-wire drift chambers tracking linear particle trajectories. The algorithm developed used a simple two-dimensional adjacency based on a track's front and back intercepts in the detector. A variant in which the adjacencies were dynamically created during the discovery of potential tracks was also evaluated. These were compared to a previously implemented algorithm which instead used the underlying detector hits to group cloned tracks. The new algorithms are shown to have a linear time complexity with respect to the number of potential tracks, while still reproducing or exceeding the tracking efficiency of the more complex hit-based algorithm. Since the theoretical lower bound for clustering is linear, this approach appears to be near-optimal. Future studies are needed to assure that the results of these approaches are correct, though, as data produced from known tracks was not available to compare against. Pending such an investigation, the algorithms compare favorably against the original and could be considered for use in order to decrease the time needed for analysis of the data.

Wireless Network Monitoring Software

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Computer and network systems are crucial in a laboratory setting. With computers, researchers can model experiments without needing to perform them, store results and communicate quickly and easily with other researchers around the world. Therefore, it is important that any problems be fixed quickly so that disruptions are minimized. Argonne National Laboratory's wireless network allows users to connect to the laboratory's computer network anywhere in range of an access point (AP) without the need for network cables. However, the wireless network is as subject to failure as any other system. For this reason, the laboratory decided to develop an automated program that can test, diagnose and report problems found in the wireless network. This project was developed for the Ubuntu Linux operating system and

is written in Python. It uses Django to aid in storing and presenting collected data. Software used by the project includes WPA Supplicant, a tool used in Linux to manage WPA encryption and NDISwrapper, a utility that allows the use of Windows wireless card drivers in a Linux environment. The project has developed to the point where computers running it are able to perform tests on APs and networks including association, signal quality graphing and DHCP. The program can then take the testing data and present it on a simple web interface. A script also runs on the web server that checks all the results reported by the computers running the testing software. If a failure is found, it sends an e-mail to administrators to notify them of the failure. This project fills an important gap in computer technology because there are no readily available programs which will perform tests from the client side of networks. There are several large-scale programs that will test systems from the server end (Nagios, for example) and there are programs available that will perform simple tests from the client side, but nothing on as large a scale as this software. Ultimately, however, issues such as firmware bugs, incompatibility between Linux and the computer's hardware, and issues within Linux limited development and ensure that more work needs to be done before this software is ready for production.

Designing a Useful Browser-Based Database Interface

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Information Technology Services Division uses CFEngine (which stores its data across multiple tables in a SQL database) to administer all Unix-based computers at Oak Ridge National Laboratory. Acquiring useful information from this large database is difficult with the website-based interface currently in use because it is a simple PHP/HTML site capable of returning entries from only one table at a time. This project was to design and implement a new interface that would allow users to gather useful information from the database more quickly. The current database is being served by MySQL, so PHP was chosen again because it is easy to integrate with MySQL. The dynamic nature of a PHP page enables the generation of more complex SQL queries capable of collating data across multiple tables of the database. This approach yields more meaningful and useful result sets. I used JavaScript to employ techniques often referred to as AJAX (Asynchronous JavaScript and XML); AJAX techniques make the site behave as if it was a desktop application, which makes the site more user-friendly. The new interface improves on the original in several ways, but it does not attempt to replace it. The original interface provides search capability for individual tables and simply gives the results without cross-referencing tables. The new interface streamlines and simplifies ways of visualizing the available data by bringing together, onto one page, relevant data from multiple tables (i.e., machines, users, packages, patches, etc.). The simplification aspect is that much of the information available in the database is not used. The new interface provides a much faster way to accomplish common system administration tasks, such as contacting all the owners of all systems in need of a new software patch. By using the two interfaces side by side, administrators can quickly accomplish routine tasks without jumping between tables to look up cross-references or sort through unfiltered views of individual tables for specific needs. This new interface can be extended to provide custom data views for common tasks. These data views would need to be designed for specific scenarios. Because unpredictable circumstances are inevitable, the new interface can augment, but probably cannot replace the existing CF Engine interface.

Performance Monitoring of SLAC Blackbox Nodes Using Perl, Nagios and Ganglia

Roxanne Martinez (STANFORD UNIVERSITY, STANFORD, CA 94305), Yemi Adesanya (SLAC NATIONAL ACCELERATOR LABORATORY, STANFORD, CA 94025). The High Performance Computing Group at the SLAC National Accelerator Laboratory (SLAC) monitors the laboratory servers to ensure optimal computing performance. The group uses two types of monitoring application software: Nagios and Ganglia. Currently, the software is used to track such metrics as the percentage of CPU in use, the amount of memory in use and the input/output rate of machines. The introduction of an additional 547 servers last year meant the need for additional monitoring to keep track of three metrics that Ganglia and Nagios do not monitor automatically: temperature, fan speed and voltage. The new servers are housed in two new portable computing centers, or blackboxes, produced by Sun Microsystems. By calling on the machines' baseboard management controller (BMC), users are able to print out the needed metrics. Scripts written in the Perl programming language were created to make use of this functionality and to allow

the group to monitor machine health using the two forms of monitoring software. The needed metrics were extracted from the text output using Perl for status evaluations in Nagios and Ganglia. For this project, the scripts created were first tested on three of the blackbox machines: bali0113, yili0113 and boer0113. The scripts successfully extracted the text values and correctly reported "OK" status for the three machines. The scripts were then successfully configured into Nagios and Ganglia to produce visualizations and to store the data. Now that the scripts were shown to work on the three test machines, the programs have been implemented on all blackbox nodes. This will allow the SLAC Scientific Computing and Computer Services (SCCS) group to better evaluate the blackbox cooling methods and quickly pinpoint problem areas to ensure optimal computing performance for the laboratory.

Designing an Administrative Interface for Dynamic Form Construction

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Collecting information from users via web based forms is a common method of data collection. Previously, effective forms have required direct input from skilled web designers. This project developed a system by which web forms could be quickly created and deployed. To facilitate this goal, an interface was developed which allows administrators to easily create forms dynamically. To create the interface, a combination of client side and server side technologies were used. The client portion is composed of Javascript routines and makes use of the JQuery open source library. The server portion runs an application written with the Python-based Django framework. This application supports the interactive form designer displayed on the client's web browser. Currently, the interface provides the ability to create new forms, however, much work remains before the system will be ready for production. To further the usefulness of the system, the interface needs to maintain existing forms in addition to its present capabilities.

An Investigation into Bayesian Networks for Modeling National Ignition Facility Capsule Implosions

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Bayesian networks (BN) are an excellent tool for modeling systems with several interdependent variables. A BN is a directed acyclic graph and consists of a structure, or the set of directional links between variables that depend on other variables, and conditional probabilities (CP) for each variable. One can represent various physical properties of National Ignition Facility (NIF) capsule implosions as variables in a BN. A dataset containing simulations of NIF capsule implosions was provided. The dataset was generated from a radiation hydrodynamics code. Relevant knowledge about physical properties of NIF capsule implosions and greedy search algorithms were used to search for hypothetical structures for a BN. The structures were ranked according to their marginal likelihood. After an optimal structure was found, the CP's for each variable were estimated with maximum likelihood estimation. Our preliminary results found a few important links between variables in the dataset. One link showed that the fraction of high energy (17–22 MeV) neutrons (one of the dataset variables) depended on the imploding capsule's entropy. A stronger link showed that the time of implosion depended on the imploding capsule's velocity. However, we only found seven links between the sixteen different variables in the dataset. Since there should be more links between the dataset variables based on the physics of NIF capsule implosions, the paucity of links is most likely due to the relatively small size of the dataset and the sampling of the values for dataset variables. Another factor that might have caused the paucity of links is the fact that in the dataset, 20% of the simulations represented successful fusion, and 80% did not, (simulations of unsuccessful fusion are useful for measuring certain diagnostics) which skewed the distributions of several variables and reduced the number of links. Nevertheless, by illustrating the interdependencies and conditional probabilities of several parameters and diagnostics, an accurate and complete BN built from an appropriate simulation set would provide uncertainty quantification for NIF capsule implosions.

Importance of Managing Alerts for SharePoint Users

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Being able to instantly communicate within a team and exchange important files quickly and easily is becoming a must. With the help of portal software such as Microsoft Office SharePoint Server 2007®, companies are readily able to maintain a centralized meeting ground to hold discussions, make important announcements and exchange

files. This ability to house vast amounts of information can be a curse as well, allowing a user to easily become lost. SharePoint utilizes an alerts feature for this very reason, which allows a user to receive an email based on if an item of interest is added or updated to the site. Current management for such alerts however is not as effective as it could be. The task was to help create a more robust method to manage alerts, which required 1) that a user could be selected and all the alerts for that user displayed and 2) that a list or document library could be selected and all the alerts for that list or document library would be displayed. The work involved creating a web part that would fulfill these requirements and allow a user to delete, add, or even recreate an alert based on the information presented. The web part also needed a user-friendly interface which required the addition of Asynchronous JavaScript and XML and integration of SharePoint Cascading Style Sheets classes. This allowed the application's look and feel to be much more pleasant. After thorough testing, a finalized product has been attained. With this new application, a user can manage alerts much more efficiently than with SharePoint's standard alerts manager. As newer software versions emerge, the alerts manager will require upgrades in order to maintain the effectiveness and usability of the product. Software can quickly become outdated and will always need upkeep.

Human Interface of Portable Touch Screen Devices

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Apple's iPod Touch has many features that can be used to develop a variety of applications. By analyzing the open source data and working with the Apple Developers Connection, the iPod's capabilities can be expanded. The main area of interest in this research is to create an application that utilizes accelerometer data to navigate within a virtual world. This application would relay the variance of the direction and acceleration in the (x,y,z) coordinate frame to the virtual environment to enable user navigation. Such an interface would provide a better user experience for moving in a three-dimensional computer-generated world than traditional tracked navigation devices. Further research is needed on this subject to understand the optimal way to transfer data from the iPod to a third-party application, which, for the purposes of this research, is VE-Suite, an open source virtual engineering toolkit. Additional research is also needed to support the development of multiple windows rendering applications for the MacOS platform. Specifically, extended support is needed for NSOpenGLView Cocoa window support. The virtual environment in which the accelerometer will be implemented will project onto twenty-four 30" Mac displays driven by three Mac Pro computers. However, when constructing views on separate windows or monitors, errors halted the graphics application that was driving the monitors. The proposed solution, which is still under investigation, shows that an NSRect function, which was absent in the original software application, is needed to drive multiple OpenGL contexts on multiple graphics cards. Adding and implementing this functionality will enable a multi-context rendering window application to utilize graphics cards in a Mac Pro to enable the full use of the twenty-four 30" Mac displays.

Using Web Data Extraction to Estimate Attack Risk

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The US Department of Homeland Security is quantifying the attack risk against U.S.-based chemical facilities. The objective of this study was to create a Java smart-search tool to gather information from news items in Google about chemical terrorism attacks. The expected outcome includes the smart-search Java software; lists of smart-search items (e.g., U.S. cities with population over 100 000); summary table of chemical-attack features (time, location, chemical, deaths, injuries, damage in dollars); and an estimate of risk for the various DHS chemicals of interest. To calculate the risk of chemical attacks, the smart-search tool must locate, organize and parse news items from the Internet. The specific methods involve: (1) entry of specific search terms (e.g., "chlorine attack"); (2) automated search with the terms via the Google search engine to obtain URLs for specific news articles; (3) automated extraction of text from each URL into a separate file; (4) search of each text file from for relevant keywords (e.g., "deaths" or "injuries"); (5) tabulation of the data into a summary; (6) analysis of the summary to quantify event occurrence frequencies; and (7) creation of statistical summary to quantify threat, vulnerability and consequences. Along with regular expression pattern matching, step (4) uses an open-source, full-featured text-search engine library called Lucene, which annotates and indexes the text for subsequent extraction of relevant information via proximity searches. The main results include the following: (a) an automated knowledge-discovery

methodology that obtains quantifiable information about terrorist attacks on chemical facilities; (b) implementation of that methodology in Java; and (c) sample results that demonstrate the method's usefulness. These results will be incorporated into an existing knowledge warehouse for determination of each facility's risk of a terrorist attack. Moreover, this information helps DHS chemical inspectors who will visit facilities for assurance of regulatory compliance and for preparedness improvements in terms of lessons learned from terrorist events.

Performance Analysis of MADNESS on Jaguar

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MADNESS is an environment for prototyping and developing scientific applications using multiresolution analysis and low separation rank methods. Programs written to operate in MADNESS generally are designed to run on massively parallel, leadership supercomputers, such as Jaguar, the CrayXT4 at ORNL. In parallel computing, a program is broken into parts for processing independently. This way each process does not run in series, waiting for one job to complete before starting the next job. In this manner, machine resources are leveraged and time-to-solution is reduced by several orders of magnitude. For effective parallel processing, it is imperative to know how much of the available work should be assigned to each independent process. To determine what parts of MADNESS needed the most resources, I used an example program and a performance analysis tool called CrayPat; this tool was developed by Cray Inc. for use on their machines. CrayPat is used in a sequence of steps. The first step is to compile the original source code with CrayPat loaded, so the instrumentation used to trace parts of the program can be inserted in the executable file. Because I needed to obtain specific information, it was often necessary to instrument parts of the program that CrayPat did not instrument automatically and to create some user-defined, instrumented regions within the code. These implementations allowed me to determine exactly what was traced during instrumentation. Once the code had been compiled with CrayPat instrumentation, I created the instrumented executable. I ran the instrumented executable and examined the output created by the instrumentation tools. CrayPat produces large quantities and types of data, including call trees, number of calls, time spent in functions and much more. These data allowed me to determine what portions of the program were using the most resources and taking up the most time. With this information, it was possible to identify implementation and load-balancing errors that slowed overall rate of computation. MADNESS requires much additional modification before being widely useful for scientific applications. Further tests using a larger number of processors and other methods for message passing are needed to determine what configurations work best with MADNESS. The work done on performance analysis was a large forward step for the project and a catalyst for future research.

Using The Grid Remote Application Visualization Interface (GRAVI) Services in a Taverna Workflow

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Service oriented architecture replaces local computer applications with applications offered as a service over the web. Scientific applications that are costly or difficult for individual scientists to run locally can be offered as services hosted by larger scientific organizations. Also, data can be shared through services. The distribution of scientific applications and data over the web has been called service oriented science. The focus of this project is to present a service-oriented workflow which analyzes genes, replacing functionally-equivalent workflow that the biosciences group at Argonne National Laboratory ran in the past using local Perl scripts. INTRODUCE is a Globus Incubator project being developed to simplify and accelerate the creation and deployment of web services. The grid Remote Application Visualization Interface (GRAVI) is an extension to INTRODUCE which allows users to specify a binary or executable code while creating a service. In this project, the biology tools and scripts were wrapped as services using the GRAVI extension to INTRODUCE, with subsequent deployment on a Globus web container. The workflow was built around the web services in the Taverna workflow management software. The project is advantageous because a shift from local processing to processing using web services can distribute computing power and allow data and applications to be easily shared with other scientists. For example, with INTRODUCE, GRAVI and the caGrid Metadata extension, a binary can be wrapped as a service and registered with an indexing service. This effort demonstrates that services created with the GRAVI extension for INTRODUCE can be used together in a workflow created in Taverna. This workflow is the first step in the ultimate goal to facilitate service-

oriented science in a distributed fashion that allows scientists to share data and computation power and accelerate scientific development. However, it is only a first step. An effort to further improve the workflow is still needed.

SNS Data Reduction

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Experiments conducted at the Oak Ridge National Laboratory's Spallation Neutron Source (SNS) can produce large quantities of data, which must be processed to remove as many artifacts as possible. This key process is called data reduction; it is performed using a three-tiered software architecture developed by the Scientific Computing Group (SCG) at the SNS. Shortening the execution time for data reduction would be of significant benefit to SNS users. In an effort to produce reduced data in a timely manner to the investigating scientists, one of the three tiers, referred to as the SNS Common Libraries (SCL), was selected for processing by parallel computing. I applied the techniques and code of the OpenMP parallel-processing directives to the C++ function code in the SCL. I used a SCG multi-core Linux data analysis server to compile and test the code. The code was compiled with the GNU Compiler Collection version 4.3.1, which contains support for OpenMP version 2.5. I also wrote several test programs that reduced program execution time using OpenMP directives. The application of the OpenMP directives to the SCL did not result in an appreciable decrease in the overall execution time needed for data reduction. Also, OpenMP does not support the SCL C++ idioms well: it is better suited for C and FORTRAN code. The lack of C++ exception support would require extensive recoding of library functionality to make the error handling process compliant with OpenMP. My research shows that overlaying OpenMP directives onto the SCL code does not reduce execution time for data reduction; further, it increases the need for code restructuring and may reduce clarity. I am currently exploring an alternative strategy: that of applying parallel computing at a higher tier in the architecture using the Message Passing Interface (MPI) libraries. This approach potentially will solve some of the issues and result in a faster and functional SCL.

Electrical Equipment Inspection Program (EEIP)

Cruz Peregrina (CONTRA COSTA COLLEGE, SAN PABLO, CA 94806), Keith Gershon (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). Common electrical consumer products are usually tested and certified by a Nationally Recognized Testing Laboratory (NRTL) such as Underwriters Laboratories (UL). However, at a Department of Energy national laboratory such as LBNL, we use equipment that is custom, one of a kind, or foreign made. If the equipment has not been tested and certified by an NRTL, how do we know it is safe to use? In order to provide a degree of safety acceptability, and to comply with the requirements of the Occupational Safety and Health Administration (OSHA) and the National Electric Code (NEC), LBNL has created the Electrical Equipment Inspection Program (EEIP). Over a time period of ten weeks, 367 uncertified pieces of equipment were identified to not be NRTL approved. Of the 367 uncertified pieces of equipment, 89 were inspected and, out of the 89 pieces of equipment inspected, 35 failed inspections while 54 passed. Our findings show that about 39% of the equipment may not be acceptable upon the first inspection. EEIP provides LBNL trained personnel to survey, inspect and record equipment that has not been approved by an NRTL. Furthermore EEIP also allows for any damaged equipment to be brought to the attention of the responsible individuals or groups. EEIP ensures that LBNL provides its employees with safe electrical equipment. It is estimated that it will take a concentrated effort over four years to inspect all existing LBNL electrical equipment. EEIP will increase the level of electrical safety, but ultimately, all lab employees are responsible for the safe use and maintenance of their equipment.

Babel Toolkit (Batooki)

Monica Porche (CENTRAL STATE UNIVERSITY, WILBERFORCE, OH 45384), Thomas Epperly (LAWRENCE LIVERMORE NATIONAL LABORATORY, LIVERMORE, CA 94550).

Babel is a tool that supports interoperability among computer languages widely used in science, such as C, C++, Java, Fortran and Python. It allows the creation, description and distribution of language-independent software libraries. However, Babel users have frequently requested that Babel provide a library of basic data types and common functions. The goal of this summer project is to design and implement a basic Babel Toolkit (Batooki). There are three initial elements required for the toolkit: a hash table, a command line option parser and a configuration file reader. The toolkit was written using an incremental approach. First, a map interface was created in SIDL (Scientific

Interface Definition Language). Following this step, the hash table class was defined using SIDL and also implementing the map interface. Next, this hash table class was implemented in C, using a previously created hash table. Following the hash table implementation came the defining of the command line parser class. This class also implements the map interface created earlier. The command line parser required new C code as well as the hash table created above. Subsequently, the configuration file parser class was defined in SIDL, implementing the map interface. Finally, the implementation of the configuration file parser was written in C using the hash table. With the completion of all of the steps, Babel now has a basic toolkit that allows anyone easy access to basic data types and configuration capabilities.

*** Hand Recognition System**

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One of the most significant identification technologies deals with biometrics that involves the identification of people in association with their biological characteristics. The Hand Recognition System is one form of biometrics that can be used separately or can be integrated into the (IBRS) Integrated Biometric Recognition System developed by the Brookhaven National Laboratory (BNL), the Institute of Applied Physics at the Russian Academy of Sciences, as well as Excom Inc. Its main objectives deal with securing protected objects, the control of access of people to protected objects in limited-access rooms, as well as uses in anti-criminal and anti-terrorism warfare. While many commercial biometric systems have been developed which encompasses a single biometric, the IBRS is a platform-independent program that allows for the coalition of several biometric technologies, including hand, fingerprint, face and voice Recognition Systems (RS). In order to test for effectiveness, the goal of this summer's project, the system needs to identify, as well as verify, a person or persons correctly. Several problems arose however throughout the testing process. One dealt with the incompatibility of the older IBRS system with newer versions of the Hand RS system, causing a need to revert to the older, more limited versions. Issues that arose when testing involved the image criteria. In order for a hand image to be accepted into enrollment, it must fit certain criteria, such as lighting and hand placement. The difficulty came about when the IBRS system was accepting an image and the Hand RS system was denying the image and throwing an error. This was primarily due to a bug in the system. New testing needs to be done with both biometric systems when the new IBRS is completed at a later date.

Lattice Boltzmann Modeling

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This project investigated the potential and limitations of a type of fluid simulation known as Lattice Boltzmann Models (LBM), a class of the larger field of Computational Fluid Dynamics (CFD). Traditional CFD methods model viscous fluid flow by approximating solutions for the governing Navier-Stokes equations. Yet solutions to the nonlinear partial differential equations come at high computational expense. The LBM can improve the performance and scalability of fluid flow simulation by reducing the complexity of the modeling algorithm. The method hinges on three key simplifications: (1) use of the discrete Boltzmann equation rather than the Navier-Stokes equations; (2) approximation of the continuous collision operator with a relaxation term; and (3) discretization of particle position and velocity with an imposed lattice grid. The model produces stability at flow equilibrium after a large number of repetitions in particle streaming and collision. The LBM method is attracting interest for use in many applications. Given its advantages, study is needed to establish its ability to simulate complex fluid-flow systems. In this project, I evaluated a LBM implementation written in Fortran 90. The results were visualized as animation streams of discrete time steps using rendering software (ParaView 3.2). I focused on simulating Poiseuille fluid flow over a large range of parameters and compared results with values reported in the literature. I also investigated the origins of instability (both the theoretical limitations and the implementation errors). Results indicate that the LBM code can reliably simulate fluid flow for cases within the range $Re < 100$, $u_p(\max) = 0.1$, and $\mu(\min) = 0.01$. However, instabilities increased with Re values up to 100, at which point fluid flow around an obstacle should have developed vortex shedding. Simulation of this class of higher Re values was unstable: despite some success, results in this range deviated from those reported by others. Overall, this project yielded encouraging results for the LBM approach: the code correctly demonstrated stationary vortices and some turbulence. Additional work is needed to verify the accuracy and reliability of simulations at high (>100) Reynolds numbers. Possible solutions and

lines of future work include: (1) redefining boundary conditions with more complex and consistent algorithms and (2) altering the relaxation term to depend upon local states (entropic LBM) to allow more extreme simulations.

Integrating Modeling Projections: Adding Cartographic Support to FRAMES

Gregory Sarafin (SUFFOLK COUNTY COMMUNITY COLLEGE, SELDEN, NY 11784), Mitchell A. Pelton (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352).

Framework for Risk Analysis Multimedia Environmental Systems (FRAMES) is modeling software that integrates disparate models that assess environmental factors to yield ecological impacts. Multimedia Environmental Pollutant Assessment System (MEPAS), a predecessor to FRAMES, was a collection of different environmental models. When the FRAMES project started, it integrated MEPAS, as well as other disparate models, to show its Plug and Play manner. FRAMES currently outputs this data in a textual or graphical form, but is limited in its ability to output data in cartographic form. A cartographic viewer would allow the data to be output onto a satellite image or a Geographic Information Systems (GIS) map. This lack of a cartographic viewer makes the data more difficult to interpret. By using Proj4, a cartographic projection library, FRAMES data can be translated from a Cartesian grid to geographic coordinates. These coordinates can then be placed in a Keyhole Markup Language (KML) file, a native Google Earth file, to display geographically other attributes of the data such as concentrations, release time and location.

Mac and PC Performance Analysis

Dain Schroeder (BIG BEND COMMUNITY COLLEGE, MOSES LAKE, WA 98837), Charlie Verboom (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720).

Over the course of the past year, the desktop environment at Berkeley Lab has been impacted by improvements in hardware and changes in operating system software. The performance of a computer is based on a combination of the operating system being used and the computer's hardware. In order to evaluate the contributions of these different factors, benchmarking software was used on the systems. The benchmarking products used were GeekBench, from Primate Labs, CineBench, from MAXON, (cross-platform) and PerformanceTest, from PassMark (only available for Windows). A recommendation for a single lab benchmark product was not made, because each one employed unique criteria, thus making it difficult to select a "best" tool. Experiments were done on a variety of common desktop and laptop systems from Apple, Dell and MPC. These systems spanned the range of processors from the older Pentium 4 through the latest Quad Core Xeon processor. Research validated the expectation that hardware makes a significant difference on computer performance. The research showed that the fastest operating system on an Intel Mac was Mac OS X Leopard, which was a full 15% faster than Windows Vista on the same hardware. In addition, Windows Vista is not significantly slower than XP, based on the results of the selected benchmarking tools used in this research.

*** The Active Remote Sensing of CLOUDS Statistics Value-Added Product**

Robyn Short (TIDEWATER COMMUNITY COLLEGE, VIRGINIA BEACH, VA 23453), Victor A. Cassella (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). The Active Remote Sensing of CLOUDS (ARSCL) Value-Added Product (VAP) consists of a series of code modules that manipulate data from active remote sensors to objectively determine cloud characteristics such as height distributions, radar reflectivity and vertical velocity. The ARSCL Statistics (STAT) VAP isolates and manipulates only the significant values from the ARSCL output data to produce statistics of 10-second and 30-minute frequency distributions of the liquid water path in clouds, number of points with a measurable reflectivity and cloudy points, cloud reflectivity and thickness distributions, number of clear and cloudy profiles and frequency of precipitation. These statistics are numerically transferred to data files for further analysis and also as graphs for quick overviews to use in discerning data of interest. The ARSCL-STAT program, the first of its kind, has gone unused for years because it still needed some final debugging to become fully and accurately operative. This summer I set out to resolve these bugs and make further improvements. To start, after a quick review of the code revealed a bug that contributed to inaccurate data storage, I resolved the issue successfully. Additionally, I made further corrections and improvements to this VAP using C programming, C-shell scripting and Interactive Data Language. Now that the ARSCL-STAT package has been debugged successfully and contains added features that improve the look and feel of the program, it will finally be run using the ARSCL data collected from all five Atmospheric Radiation Measurement (ARM)

sites, dating back as far as 12 years. This will establish a working data set for the ARSCL statistics. After this initial catch-up run, the ARSCL-STAT program will be run monthly to update the data. The results of these data runs will be made available on the ARM web site for public access and use. After this summer session concludes, future work to be done on ARSCL-STAT includes further statistical analysis on monthly, seasonal and yearly time scales.

Document Clustering on the Graphics Processing Unit

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Analysts are continually faced with the extremely difficult task of extracting desired data from thousands to millions of documents at a time. Our research focuses on assessing parallel approaches on a new platform, the Graphics Processing Unit (GPU). One method we evaluated borrows from nature, imitating the flocking behavior of birds. Each bird represents a single document and flies toward other documents that are similar to it. A limitation of this method of document clustering is its complexity. As the number of documents grows, it becomes increasingly difficult to receive results fast enough to be useful. Another solution, Affinity Propagation, clusters data using matrix operations to find a document's "exemplar." After enough documents have voted for their exemplar, clusters emerge as multiple documents pick the same exemplar. Flocking behavior and Affinity Propagation, along with other naturally inspired algorithms such as ant colony optimization and particle swarm optimization, are highly parallel and have achieved increased performance on expensive cluster computers. Recently, the GPU has received attention for its ability to solve highly-parallel and semi-parallel problems much faster than traditional sequential processors. Some applications achieve a huge increase in performance on this new platform. The cost of these high-performance devices is also relatively low, compared with the price of cluster machines. Using the CUDA platform from NVIDIA, we developed a document flocking implementation to run on a NVIDIA GEFORCE 8800 GTX graphics card. We also developed a similar but sequential implementation of the same algorithm that could run on a desktop CPU. We tested the performance of each on groups of news articles from a standardized document set containing from 200 to 3000 documents. Performance gains achieved using the GPU approach ranged from 36X to nearly 60X compared to our CPU implementation. Our results also confirm that each implementation is of similar complexity, confirming that gains are from the hardware: they were not from algorithmic changes. This improvement in runtime demonstrates that the GPU is a powerful platform for document clustering analysis. Our research on Affinity Propagation as a GPU document clustering solution is ongoing; preliminary results are encouraging.

Developing a Graphical User Interface for the PARCS Reactor Core Simulator

Joshua Steinberg (BUCKNELL UNIVERSITY, LEWISBURG, PA 17837), Peter Kohut (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

The Purdue Advanced Reactor Core Simulator (PARCS) predicts the power distribution in nuclear reactor cores when they are subject to changes such as the movement of control rods or changes in coolant conditions. The inputs of the program are located in a text file that needs to be completed in order to successfully achieve a working model. Some of the inputs include the core type, core power, initial boron concentration, cross-section information, fuel assembly locations and print options. Currently, the process to adjust the inputs for each of the successive simulations is a long and tedious one. A graphical user interface (GUI) has been developed to make the input of the PARCS system easier to handle for the user. Prior to this research and development, there was no GUI for these inputs. JAVA, a platform-independent, free programming language was chosen to develop the GUI. A tabbed window was created, with one tab corresponding to each input section, to make the layout of the GUI compact and practical. The inputs questions within each section (tab) are to be answered using true/false type buttons and text fields. The inputs are sent to a file to be read in by PARCS. Although the GUI is operational, there is room for further work. The code is quite long and could be made more easily readable. In addition, it would be useful to have a graphical representation of the reactor core on some of the tabs. This is particularly evident in the geometry input section and doing so would make the GUI more user-friendly. It is evident that this GUI will speed up the process of modeling the power distribution in nuclear reactor cores.

Creating Open Source, Generic, Dynamic Forms for Universal Application

Scott Thompson (EDINBORO UNIVERSITY OF PENNSYLVANIA, EDINBORO, PA 16412), Craig Stacey (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). Many administrative tasks involving user interaction (data entry) can be both repetitive and inefficient. Web-based forms collect data quickly, but a good form requires expensive technical and artistic input. An easy interface to quickly create and serve internet-based forms and databases would save a great deal of time and money. This project explored how to serve varied internet form requests through a single web server interface with minimal administrative effort and developed that interface into a working system. Different data representations were compared, from traditional database structures to query-based and non-relational systems, and prototypes of each were created. It was determined that an existing Open Source Object-Oriented framework called Django would meet these requirements if modified for some code generation. The technique for this system was developed and implemented into a working prototype; the application that resulted is a generic, internet-based system that dynamically manages forms and collects data. Forms created by this system are intentionally generic, but can easily adopt either a common look and feel or unique detailed customization through Cascading Style Sheets. Further development will occur in the near future with the intent of a public release under an Open Source license. This system provides a time-saving tool of nearly universal application; anyone collecting web-based user input could easily, rapidly and inexpensively deploy this system.

Simulator Performance Evaluation Using Benchmark Applications

Clayton Thurmer (OBERLIN COLLEGE, OBERLIN, OH 44074), Kalyan Perumalla (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Discrete event simulation is a concept used to model complex systems by scheduling events chronologically. It is used to model queuing situations, such as customers waiting for available tellers at a bank. Large-scale applications include models used for emergency event planning and response. Discrete event simulations are characterized by their scale (several millions of simulated entities), fine-grained nature of computation (microseconds per event) and highly dynamic event interactions. Synchronizing events is the primary challenge. For this project we compared two discrete event simulator packages: SimScript 3 (a commercial product distributed by CACI Corporation) and *psik* (music; an open source simulation engine developed by Kalyan Perumalla). The object of interest in this comparison was the scalability of the simulators with respect to speed and memory requirements when the model size is increased from a small number of simulated objects to thousands or millions. We used two benchmarking applications to evaluate and compare performance. PHOLD is a common discrete event benchmark in which simulated players schedule events for other players at random intervals into the future. Events must be executed in timestamp order, regardless of the destination or source player. This benchmark was implemented previously for *psik*, and therefore was the first application chosen for development in SimScript. An efficient version of PHOLD was implemented using the global event queue provided by SimScript primitives. Scaling experiments using PHOLD show *psik* with fewer microseconds per event than SimScript for most trials (up to 220 players). A second, more complex, benchmark was developed for both simulators. This benchmark is a model of civilian violence that uses an agent-based approach. Agents move throughout a grid and determine whether or not to "rebel" based partly on information about their neighboring grid cells. "Cop" agents also populate the grid and "arrest" rebelling agents by removing them from the simulation for several iterations. We used object-oriented programming to encapsulate the grid and prevent inconsistent states. This model was implemented for both simulators and was compared to published results. A graphics component was also added to the SimScript version. *psik* had smaller elapsed times than SimScript during trial runs of the civilian violence model. We generally found that *psik* outperformed SimScript in the benchmark evaluations.

Search Engine Optimization on ChemAlliance.org

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Google has 70% of the search engine market share in the United States and an even larger share in Europe. This commanding share alone makes it necessary to optimize websites specifically for Google if websites expect to receive visitors from it. ChemAlliance.org, a website dedicated to chemical regulations information, was chosen as the target website to optimize. Various strategies were used in the optimization and all of the strategies can be used on any other website. Inbound links were analyzed and external websites were contacted about links

to ChemAlliance.org. New organization features were implemented and information was strategically relocated. Website code and HTML was updated to ensure compliance with W3C standards. Google Analytics, Google Webmaster Tools and local server logging software was used to collect data about visitors and traffic before and after optimization changes were made. When the two data sets are compared few significant changes are noticed. An increase from 91.16 to 109.5 visits/day was the most significant and positive change. The results indicate that the techniques used do not cause immediate results, but more time would be needed to see any larger significant results. There were no significant negative results. The techniques were practical and free to implement, making any positive effects a success.

Software Tool for Simulating Multiple Sensor Detections

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Intrusion detection is an important aspect of infrastructure security. Physical security measures, such as electronic locks and physical contact sensors, are often used for this purpose. However, once an intruder breaches these security measures, he or she is within the secured area and can carry out a malicious objective. Thus, there is a need to detect intruders outside of the secured perimeter. Perimeter surveillance radar system (PSRS) units are well suited for this role. However, the command and control operator's display becomes quickly cluttered with redundant data in an operational environment. Therefore, Pacific Northwest National Laboratory (PNNL) is developing software that uses a correlation model and GPS radio frequency (RF) tags to solve this problem. It is necessary to test the software's ability to handle different detection scenarios. Therefore, a software tool should be developed that can directly supply simulated sensor detections to PNNL's software. Although the commercial sensor systems do provide simulation software capable of generating sensor detections, they do not provide the necessary tools for generating both radar and RF tag detections. Therefore, a new software tool was developed that can do linear interpolation, with stochastic error, on a set of existing geodetic sensor detections. The results of the interpolation become a newly generated track of sensor detections. This tool integrates with PNNL's software using eXchange markup language (XML) that complies with the ICD-0100 standard published by the Security Equipment Integration Working Group (SEIWG). The simulator provides a useful tool for PNNL to create and run custom test scenarios for their existing software without the need to conduct a field exercise for every test. The tool also allows for the augmentation of recorded field test data with new or modified sensor tracks, and it can create a large number of detections for scale-up testing. Although useful, the graphical user interface is very cumbersome and future development should focus on creating a more intuitive interface.

Chemical Infrastructure and Information Availability

Ben Winter (MIDDLE TENNESSEE STATE UNIVERSITY, MURFREESBORO, TN 37132), Lee M. Hively, Ph.D (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831).

The Department of Homeland Security (DHS) has the mission of protecting the chemical infrastructure of the United States. Oak Ridge National Laboratory is constructing a knowledge warehouse, which will include chemical information and specialized tools and algorithms that aid inspectors in planning and performing site inspections. The knowledge warehouse also will provide a comprehensive resource for subject-matter experts to support the chemical inspectors. This project involves analyzing subject-matter coverage from many sources, constructing a repository, associating the information with DHS chemical security issues, and designing and implementing a repository. I constructed an information-availability matrix to assess the information completeness across the sources currently available (both online or hardcopy). This matrix depicts the degree of information fragmentation and the extent of completeness across the disparate sources, showing the need for a comprehensive repository to support the chemical inspectors. Consequently, a repository was constructed. A logical model of the information and the inter-relationships to be included in the repository was produced using an entity relationship modeling tool, which was then converted to a physical model and implemented as an Oracle schema. I then populated this schema using standard Oracle and Microsoft tools. Because of the complexity of the metadata to be saved, a graphical user front end was required to expedite information collection and storage; I created preliminary mockup screens for that interface. Use-case scenarios and requirements were defined for the information software, as well. The net result of this repository design and construction effort was 35 normalized tables, of which 28 are now populated. This project provides a first-of-a-kind knowledge warehouse of chemical information and tools in one easily accessible collection that

previously existed only as fragments in multiple places. This knowledge warehouse will support site inspectors, subject-matter experts and DHS in efforts to protect chemical facilities from terrorist attacks.

Ligand Investigation

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There have been many studies of ligands (small molecules) that bind to protein molecules. Although the identification of ligand structures has been performed for many years and over 8800 structures have been deposited in databases, there are many variants of the same structure, complicating the use of the overall ligand list. The goal of this research is to create a list of the top 200 most commonly found ligands. Crystallographers who study protein crystals may have a ligand in their protein that is significant to their research direction. This new list will cover over 60 percent of ligand entries and will increase the probability of ligand identification. Searching the protein database (PDB) provided information that helped categorize the ligands. Methods that enumerated the list included using graph methods to compare and contrast ligands topologies. In addition, the PDB was searched to find the ligands with the most PDB entries. In doing so, a programming language, Python, was used to speed the process. Additional studies will use Python-based Hierarchical Environment for the Integrated Xtallography (PHENIX) suite of codes. This new software will provide essential algorithms to be carried out to process reduced intensity diffraction data into refined molecular models. Moreover, this software can create structures that will help enumerate the ligand list.

Using Machine Learning Algorithms to Predict Protein-RNA Interfaces

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RNA-Protein interfaces are important subjects for study because of their role in protein synthesis, gene expression and virus replication. The prediction of these interfaces with machine learning classifiers, forms of computational models, is especially useful because it can aid wet-lab experimentation, saving time and money, as well as predict interface locations for proteins that are not easily studied in wet-lab. Our goal is to improve prediction of these RNA-protein interfaces. In our research, we use a dataset of 147 protein amino acid sequences with RNA interactions identified through X-ray crystallography in the Protein Data Bank. Building upon the WEKA machine learning package, we develop and implement a two-stage classifier, which utilizes a recurrent sliding window methodology. This two-stage classifier is used to exploit the correlation between the dataset's labels (interface or non-interface). The first stage of the classifier is given an amino acid and an equal number of amino acids on each side (the sequence context). The classifier is then trained to label this amino acid. The second stage is given the amino acid sequences as well as a window of the predicted labels. The second stage of the classifier is then trained to label these and to ultimately return the classifiers' final predictions. Using this classifier with the Naïve Bayes classifier, we are able, for the same precision, to improve recall rates in comparison to a single-stage Naïve Bayes classifier.

Engineering

Linking Field-Programmable Gate Arrays to Linux PC

Marcus Baines (NORFOLK STATE UNIVERSITY, NORFOLK, VA 23504), Ryan Herbst (SLAC NATIONAL ACCELERATOR LABORATORY, STANFORD, CA 94025).

The purpose of this project is to provide a high speed data link between Field Programmable Gate Array (FPGA)-based designs and a Linux PC. This is a general purpose design that will be used in many applications, with the primary target being International Linear Collider detector development. Like similar projects, the current implantation of this hardware uses a USB link between the FPGA and a PC as a data transport mechanism. This interface is limited to a throughput of around 300 kilobytes per second. There are also known bugs with the Linux driver for the USB chip which causes errors to appear periodically in some setups. As a result of this, initial tests of a 1 Gigabyte Ethernet link have shown that a data transfer rate of around 80–90 Megabytes per second can be achieved. This rate is slower than the theoretical rate of 125 Megabytes per second due to a few "handshake" issues. This project is unique in the fact that it is the first of its kind. It is broken into three pieces: the hardware interface, the software Application Programming Interface (API) and the data transfer between hardware and the software. Through the use of two program codes, C++ and Very High Speed Integrated Circuit Hardware Descriptive Language (VHDL), the hardware and software will be able to break up packages that are too large (larger than 8 KB) into smaller frames and send them over the

Ethernet, using the Pretty Good Protocol (PGP), at the theoretical rate of 125 MB per second. Also, through this protocol, the user interface will be rate matched with the Ethernet MAC so handshaking is not required from the receiver of the frames, and this should also prevent the errors that occur in the transfer process.

Performance of Military Specification Lubricant in Extreme Tribological Environments

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Military ground vehicles involved in combat operations present a particularly extreme tribological environment. This environment includes lubricant contamination by various particulate matter and loss of lubrication due to mechanical damage sustained during battle. It is advantageous for a vehicle to be able to return its occupants to safety under these circumstances. To evaluate a current MIL-L-2104 specification engine lubricant (Shell Rotella T SAE 30), two types of tests were conducted. The first involved mixing the specified oil with test dusts containing four different particle diameters (avg. diameters 4.5, 10, 12 and 30 μm) at four different concentrations (5 g/kg, 1 g/kg, 0.5 g/kg, 0.1 g/kg). These contaminated oils and a clean control oil were tested in a four-ball test rig according to ASTM D-4172. The data from these tests and an analysis of the balls using optical profilometry was used to determine friction and wear characteristics. It was observed that smaller particle sizes caused higher wear, possibly due to particle coagulation or a comparatively greater number of particles in the oil. Higher levels of contaminant loading also led to higher wear. Additionally, high contaminant loadings caused the friction to temporarily rise and then fall and stabilize at a lower level for the remainder of the test. The "oil-off" test utilized a block-on-ring rig. A 500 N load was applied, the supply of lubricant removed, and the time to scuffing failure was recorded. Various liquid and solid lubricant additives were evaluated. The most promising were Elektrion R (10:1) with an average performance increase of 73%, and molybdenum disulfide (1.6 wt%) with an average performance increase of 64%. Further research into lubricant formulation and the addition of solid lubricants should increase the reliability and robustness of vehicles in the aforementioned environments.

The Effects of Polymer Electrolyte Membrane Fuel Cell Membrane Electrode Assembly Manufacturing Defects on Cell Performance

Christopher Bochart (COLORADO SCHOOL OF MINES, GOLDEN, CO 80401), Michael Ulsh (NATIONAL RENEWABLE ENERGY LABORATORY, GOLDEN, CO 89401).

Decreasing reliance on foreign energy sources is an important goal for America. Fuel cells powered by clean hydrogen and air are one renewable energy technology being researched and developed. To get fuel cells on the market, tolerances for manufacturing must be established. This study attempted to correlate manufacturing defects with fuel cell performance so that validated manufacturing tolerances for fuel cell components can be established. Accuracy of the fuel cell testing station equipment was verified according to United States Fuel Cell Council (USFCC) protocol. Pristine and "flawed" (manufactured with a defect such as a pinhole) polymer electrolyte membrane fuel cell (PEMFC) membrane electrode assemblies (MEAs) were tested according to USFCC protocol. Ex-situ characterization of the MEAs was conducted by means of thickness, in-plane and through-plane resistance measurements and optical microscopy. The MEA was first "broken in" to fully humidify and condition the cell. In-situ characterization techniques were then employed including fuel cell polarization, hydrogen crossover and electrochemical surface area measurements. The fuel cell polarization curves (cell voltage vs. current density) were compared to published data as well as to each other to gauge performance (Cell voltage at 0.8 A/cm²: BASF published=0.68 V; Pristine MEA=0.54 V; Flawed MEA=0.45 V). It was found that the flawed MEA performed worse than the pristine MEA. Hydrogen crossover data showed conclusively that the flawed MEA with the pinhole experienced significant hydrogen crossover while the pristine MEA did not (11.4 and 0.7 mA/cm² respectively), as expected. However a greater than acceptable high frequency resistance (HFR) was observed (100 m Ω ·cm² is acceptable while 150–400 m Ω ·cm² was observed) for the MEAs. The high HFR paired with a lack of repeatability of results due to time restrictions (resulting in the testing of only one pristine and one flawed MEA) does not allow for a conclusive statement to be made at this time concerning the effects of PEMFC MEA manufacturing defects on cell performance. Further studies in which repeatability of results can be established (while decreasing the HFR) using multiple pristine and multiple flawed MEAs are required to effectively correlate the effects of MEA manufacturing defects on cell performance.

Arc Flash Analysis Project

John Boucher (MIDDLEBURY COLLEGE, MIDDLEBURY, VT 05753), Alan Raphael (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

Before an arc flash accident prompted Brookhaven National Laboratory (BNL) to devise the Arc Flash Analysis Project (a project designed to achieve a complete electrical systems analysis of all BNL systems and buildings), many of BNL's older facilities had not been inspected to determine if they satisfied the National Fire Protection Association's "Standard for Electrical Safety in the Workplace" (NFPA 70E-2004). For the Arc Flash Analysis Project, equipment layout and manufacturing and operating information for all electrical components such as panels, fuses and circuit breakers, as well as cable sizes, types and approximate lengths was obtained by manually inspecting and tracing out the facilities' electrical systems. Using SKM PTW Power Tools Software (PTW), this information was organized, illustrated and then analyzed to establish the electrical systems' susceptibility to and energy available for arc flash. The work done for this study produced single-line electrical diagrams containing all electrical equipment down through the lowest rated panels (480 Volt or 208 Volt) to any three phase 480 Volt or three phase 208 Volt/225 Amp or greater equipment. PTW was used to compute information such as arc flash incident energy level at each equipment location, the flash protection boundary and the recommended Personal Protective Equipment (PPE). This study sought to achieve greater safety for those working on BNL electrical systems by providing recommendations for necessary PPE for electrical workers, collecting data to be archived, managed, updated as necessary and made accessible to facility engineers for future electrical work and affixing up-to-date arc flash warning labels to all appropriate electrical equipment.

Net Zero Energy Community: A Preliminary Evaluation

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As a result of concerns over the security of the national energy supply and the adverse environmental effects of traditional power generation, the Department of Energy has developed a strategy for reducing the energy demand of buildings through its Building Technologies Program. The goal of marketable net zero energy buildings by 2025 will significantly reduce the growing energy demand of the nation's largest energy user. In general, net zero energy describes a building that produces as much energy on-site through renewable sources as it draws from the existing power grid. The concept has been applied on an individual building basis, although the benefits achieved through economies of scale suggest that an aggregate of buildings would be more apt to achieve the net zero energy goal. Consequently, a literature review was conducted to determine if any community-scale research on the concept had been undertaken. The literature review produced much information on the progress of technology development and endeavors into net zero energy home and commercial building design. Community-scale renewable energy systems have received much attention as a power solution for isolated communities. In the United States, distributed resources are clustered together as support for the traditional grid. Additionally, the introduction of solar power technologies suitable for community-scale projects promises better efficiencies and lower capital costs than photovoltaic (PV) arrays. Combining these elements holds promise for the possibility of developing a net zero energy community, which has not been presented in scholarly works or developed in the real world. Looking ahead to the prospect of exploring the net zero energy community concept, a basic outline for research has been presented that includes four components: selecting a model community, gathering initial data, sizing a renewable energy system and evaluating the theoretical system.

Roadway Condition Assessments and Traffic Flow Studies at Argonne National Laboratory

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Roadway conditions decline over time as a result of age, load application, traffic amount, weather and climate. The 27.3 miles of roadways at Argonne National Laboratory require yearly maintenance to ensure the safety of drivers. This maintenance can range from filling a pothole to routine crack sealing. However, normally only the main roadways receive this maintenance. This project focuses on the conditions and classifications of the roadways, and what needs to be done in order to repair them. The majority of roadways at Argonne are over 20 years old, and most of those with an age in excess of 35 years are in very poor to near-failure condition. In order to determine which roadways are in the most peril, each Argonne roadway was assessed according to the roadway distresses involved and the type,

volume and severity of each distress. From that assessment data, a Pavement Condition Index (PCI) value was calculated. In addition, a pneumatic traffic counter was placed on each main section of roadway, and the data collected was used to classify that section as major, minor, local, or low-use. Priority was then determined by combining the PCI and the classification. The overall average PCI reflects that most roadways are currently in need of reconstruction or will be in need in the coming years. The traffic counts provide conclusive evidence that certain roadways, such as Watertown Road, can be closed down during the wintertime to help save on costs of salting and snow plowing. By calculating priority values, roadways such as Westgate Road are deemed to be in peril and must be repaired.

Evaluation of the Catalytic Performance of Copper In the Oxidation of Biodiesel

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Fatty Acid Methyl Ester (FAME) made to the American Society for Testing and Materials (ASTM) standard D6751 is a renewable fuel that, when domestically produced, can decrease dependency on foreign energy while reducing harmful emissions including sulfur oxides, particulates and CO₂. FAME, commonly known as biodiesel, is often associated with natural degradation and poor stability properties. With this association, the industry is concerned that copper fuel system components will catalytically affect biodiesel degradation. The purpose of this study is to quantitatively evaluate the catalytic performance of copper fuel system components in the oxidation of biodiesel over time. It was hypothesized that with age, copper tubing used in the field would have significant coatings and deposits from previous fuel degradation that would limit the catalytic effects of copper on biodiesel through minimal surface area contact. In order to determine the catalytic effect of new copper on biodiesel, samples of 100% biodiesel (B100) were aged in tubing utilized by industry fuel systems. To age the fuel samples, a temperature controlled environment was utilized to thermally accelerate the fuel's effective exposure to the copper. The aged fuel was then analyzed through Fourier Transform Infrared (FTIR) spectroscopy to measure the change in percent of infrared (IR) absorption across the IR spectra. Through the oxidation process of biodiesel, peroxides are among the first components to be produced. Based on IR absorption signatures that specific compounds produce, it is possible to correlate an increase in absorption of IR light at the wave number range of 3500 cm⁻¹ to the formation of peroxides. The relative quantity of peroxide formation is accounted for by the total change in IR absorption. Through this technique, it is possible to determine the magnitude of oxidative degradation in biodiesel. The FTIR results have shown the catalytic performance of new copper in biodiesel is not measurable. New copper, in comparison to quartz and stainless steel, performed identically. Because of the performance of new copper, it was not necessary to test the performance of aged copper. These results have produced a broad mapping of the peroxide formation in biodiesel. From this, one concludes that the overall catalytic performance of copper is low under these conditions, and that copper component based fuel systems are biodiesel compatible.

Design and Fabrication of a Q-BPM Calibration Tone Generator for the ATF2

Ian Bullock (HARVEY MUDD COLLEGE, CLAREMONT, CA 91711), Doug McCormick (SLAC NATIONAL ACCELERATOR LABORATORY, STANFORD, CA 94025).

The Accelerator Test Facility (ATF) in Japan uses cavity beam position monitors (BPMs) attached to quadrupole magnets to determine the position of the electron beam. The beam position monitors are connected to a downmix circuit which produces a 20 MHz signal from the 6426 MHz input from the BPM. A circuit has been made to produce a switchable calibration signal that is the same frequency as the 6426 MHz signal from the BPM cavity. This circuit, which will use a 714 MHz damping ring source as its input, can then be used to calibrate the gain of the downmix electronics to provide more accurate measurements of beam position. Both SMA connectorized and printed circuit board versions of the calibration tone device were produced. Both gave a little less than 0.0 dBm output at 6426 MHz with a 10 dBm, 714 MHz input. The switch isolation for each design was found to be 90 dB or better, which should ensure that the residual calibration signal does not prevent accurate measurement of the electron bunch.

Safety Set-Point Allocation

Elisabeth Byrd (GEORGIA INSTITUTE OF TECHNOLOGY, ATLANTA, GA 30332), Dave Lousteau (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). The objective of this study was to establish a safety mechanism that will prevent a catastrophic failure due to a flow blockage, occurring primarily in the heat exchanger inside the Spallation Neutron Source

(SNS) mercury target system. The target service bay houses the mercury loop consisting of the SNS target, pump, storage tank and a heat exchanger along with various piping connecting the components. If a blockage occurs in any of the heat exchanger tubes, the pressure around the system will rise and the cooling of the mercury will be inhibited, leading to unsafe conditions. A pressure set-point will be established, based on these results, to trigger proton beam shut down if this occurs. In order to understand the effects of blockage in the heat exchanger tubing, a fluid analysis needed to be performed by modeling the mercury loop using a computer program. A flow modeling program called Fathom was used to map out the loop components. Data on each part of the loop including pipe elbows, venturies, wyes and various other components was entered into the program. An existing 3-D model of the loop, previously made using ProE, was the source of input data for the Fathom model which performed flow analysis with differing percentages of blocked tubes in the heat exchanger. Pressures at the inlet and exit of the pump were calculated based on varying percentages of heat exchanger tube blockage. A forty percent blockage results in a ten percent increase in pressure at the pump outlet. Blockage of this magnitude is created by a hundred square inch obstacle which is unrealistic. Thus, a pressure set-point will not be indicative of a heat exchanger flow blockage. Therefore, other parts of the mercury loop need to be considered for blockage. Similarly, the thermal couples in the flow do not respond significantly to blockage in the heat exchanger. The use of flow meters upstream of the target is now being investigated in conjunction with Computational Fluid Dynamics modeling of the target to convey what flow causes an unsafe rise in temperature. When designing a system, safety is always the number one concern. This research will facilitate monitoring possible blockage in the mercury loop in order to keep the loop's components from failing and the immediate area safe.

Use of Congo Red Assay and HK Assay for Cellulase Characterization

Jasmine Cancino (OHLONE COLLEGE, FREMONT, CA 94539), Masood Hadi (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). This research was undertaken to determine optimal methods to characterize cellulase. The Glucose Hexokinase (HK) Assay was used to measure glucose in solution. The performance of Congo Red Assay was used to determine the sensitivity and usefulness of the assay analyzing enzyme activity. Ramazol Brilliant Blue R (RBBR) is a dye used in Azo CMC Assay protocol. An unknown molar extinction coefficient and a maximum absorbency wavelength is to be determined. Series of concentrations of glucose were mixed with HK and inserted in the multimode detector. CMC/Agar plates of different pHs were spotted with different concentrations of enzymes and incubated for two nights. Several Concentrations of RBBR were inserted into the ultraviolet-to-visible (UV-Vis) spectrometer. The Glucose HK Assay had a positive relationship with enzyme activity vs. area. The sensitivity of Congo Red Assay was not enough to detect significant difference in enzyme activity based on pH. The molar extinction coefficient value of RBBR was $4346.3 \text{ (M}\cdot\text{cm)}^{-1}$ and the maximum absorbency wavelength is in the range from 590 nm to 597 nm. In performance of glucose HK Assay protocol, the standard graph is ready to be used for future usage with enzymes. Congo Red Assay is not sensitive enough to detect significant difference in enzyme activity.

Thermal Analysis Validation through Thermal Imaging

Manuel Castro and Guadalupe Cortes (ILLINOIS INSTITUTE OF TECHNOLOGY, CHICAGO, IL 60616), Jeffrey Collins (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). All beam-interacting components in the Advanced Photon Source (APS) require thermal and stress analyses using computer aided software prior to fabrication and installation to ensure that thermo-mechanical limits are not exceeded during operation. A common question asked is how accurate these results are and if adequate operational safety margins have been incorporated into the component design. This study was conducted to validate that the theoretical findings resulting from computer thermal simulations match the experimental findings for a GlidCop® (alumina oxide dispersion strengthened copper) block sample as it is heated by the APS X-ray source. The block is water cooled and uses wire coil inserts for enhanced heat transfer. The U-shaped water channel in the block uses forced convection to keep the block from overheating. The heat transfer coefficients for this configuration are experimentally determined as a function of coolant flow rate. The emissivity of the test piece is experimentally determined as a function of temperature, surface finish and orientation. These parameters are fed into the computer simulation model and compared to experimental results obtained at the beamline. An infrared camera is used to measure the surface temperature of the block and the

enthalpy rise of the water is measured to determine the total power absorbed in the block. When compared, the final results confirm that thermal simulations provide fairly accurate results and can be used with confidence in the design of new beamline components.

Evaluating Data Center Indoor Air Quality

Benjamin Chu (UNIVERSITY OF CALIFORNIA-BERKELEY, BERKELEY, CA 94720), Ashok Gadgil (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720).

Data centers serve an important role in storing information and computational power, but their energy demands are steadily rising. An emerging technology to alleviate this problem is an economizer, which turns off the power-consuming chillers and brings in outside air for cooling. However, contaminants in outdoor air can lower the reliability of electronics through corrosion, which can negate any energy savings. This experiment seeks to determine if the indoor air quality of economizer systems is suitable for data center use. To accomplish this, the mass concentration of the particulate matter was measured both inside and outside of the data center, using aerosol measurement instruments. Particles were captured using collection filters, to identify their chemical properties. Ionic particles are of interest because they can bridge the electrical isolation between conductors. Speciation of these aerosol constituents was done using ion chromatography. After comparison of indoor and outdoor air, it is shown that indoor particle concentrations rise when the economizer is operating, due to bringing in outside air. Despite this increase, the concentrations are well below the accepted American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) standard, which confirms that economizer use does not pose a risk for the servers in a data center. Also, higher rated filters are more effective, but not necessary to meet air quality standards when a weaker filter can still meet the ASHRAE standard.

Prototype Roof and Attic for the Residential Retrofit Market

Travis Cowart (BEVILL STATE COMMUNITY COLLEGE, FAYETTE, AL 35555), Dr. William (Bill) A. Miller (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831).

We designed, constructed and installed a prototype roof assembly to determine the energy and economic justification that would promote its acceptance in the retrofit market, when the roof is replaced every 15 years. We computed the daily and weekly energy savings for the prototype assembly versus the conventional roof assembly. Our research revealed a 90 percent drop in the peak heat transfer for the prototype roof, compared to the conventional asphalt shingle roof. The prototype roof has an expanded polystyrene insulation (EPS) with aluminum-foil facing affixed to a standard shingle base. Oriented strand board (OSB), also with aluminum foil facing, was attached (foil facing down) to the EPS insulation. Between the EPS insulation and the OSB is an air space of about 2.5 cm, which allows for natural convection to carry heat flow away from the attic. Heat flux transducers and thermocouples embedded in the roof deck and the attic floor allow measurements of thermal performance. The data were written electronically to an Excel file. Three weeks of field measurements have been completed. These measurements show that the integrated heat flow for the prototype system is about 38% less than the heat penetrating through the conventional roof and attic system. The temperature measurements showed that the EPS insulation never exceeded 38 °C. Thus, the prototype roof does not suffer the severe temperature swings that usually occur in conventional roof systems (only minor improvement through the 24-h ceiling heat ratings). However, we found, on average, a 38% reduction in heat flow for the daytime, and a 22% reduction in heat flow during the night. These results demonstrate that the prototype assembly reduces heat loss during all times of the day. The prototype roof system costs about \$250 per square (100 ft²) to install on an existing shingle roof compared to \$100 per square (100 ft²) for conventional shingles and labor (in the southeast). Annualized energy savings can be used to judge the cost premium for retrofitting a conventional roof system with the prototype system.

Use of National Instrument's LabVIEW to Create Database of Tested Batteries

Michael Cozza (UNIVERSITY OF ILLINOIS, URBANA-CHAMPAIGN, URBANA, IL 61820), John Basco (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). The Electrochemical Analysis and Diagnostics Laboratory (EADL) and Fuel Cell Test Facility (FCTF) in the Chemical Sciences and Engineering Division (CSE) at Argonne National Laboratories (ANL) provide battery and fuel cell developers with performance evaluations of their products. The current system of keeping track of the battery inventory is approximately thirty years old and the program used is outdated, causing the need for a new database program. Old

equipment is being phased out and a new way to store battery information was needed. National Instrument's Laboratory Virtual Instrumentation Engineering Workbench language (LabVIEW) was used to write the new program. LabVIEW is used almost exclusively to run tests on batteries and fuel cells, and to operate laboratory equipment. LabVIEW is a graphical computer language that uses, as the language, virtual wires connecting nodes in a flow chart, rather than using a text code common in languages such as C, Visual BASIC and Python. Each new program made in LabVIEW is called a virtual instrument (VI). LabVIEW was used to create a VI database. The new database stores battery specifications, including the battery identification number (BIN), manufacturer, dimensions, voltage and peak power. LabView proved to be a very easy and useful tool to write a program from the ground up. The VI accomplished all of the goals set out at the beginning of the project. The VI provides a user friendly database to easily access information, as well as a database that is easy to amend and edit. The VI runs seamlessly and is now what is called an "executable", or a program that can no longer be edited. The EADL and FCTF in the CSE are now equipped with this shared program. The EADL and FCTF are using National Instrument products more exclusively now, which will ensure the longevity of this battery database program.

Performance-Based Brake Tester Data Correlation

Mark Thomas Cutone (CLARKSON UNIVERSITY, POTSDAM, NY 13699), **Gary Capps** (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). On U.S. roadways approximately 42,642 deaths occurred in 2006 (preliminary data), of which 4,995 involved commercial vehicles. During an investigation from 2001–2003, 30% of all trucks involved in the study had brake deficiencies. Efforts are being made by law enforcement agencies to reduce the number of accidents involving heavy vehicles through the North American Standard (NAS) inspection program which results in 55.3% of vehicles inspected being placed out of service (OOS) because of vehicle brake issues. This study seeks to explore a possible correlation between the Performance Based Brake Tester (PBBT) and NAS Level-1 inspection results. A PBBT is a device that can assess the braking capabilities of a vehicle through the measurement of brake forces as a vehicle engages in a braking event while on a PBBT. A direct correlation could lead to the use of the PBBT machine as a major brake inspection tool. If found to be a viable, the PBBT could reduce inspection time, increase the number of vehicles receiving brake inspections, and potentially, increase roadway safety. Since July 2007, the Tennessee Department of Safety has been using a PBBT to collect data as they perform their NAS Level-1 vehicle inspections. Using this collected data, an analysis involving 277 trucks and their 2,518 wheel-ends was conducted. Based on the OOS and Overall Efficiency results, the inspections and the PBBT agreed 69.31%±5.44% of the time. Discrepancies occurred when the vehicle failed inspection and passed on PBBT, occurring 19.86%±4.7% of the time. Inspections in which a vehicle passed inspection but failed PBBT testing occurred at a rate of 10.83%±3.66%, all with 95% confidence. The wheel-end analysis resulted in a matched result rate of 67.38%. The inspection pass-PBBT fail discrepancy (P-F) occurred on average 29.9% of the time; while the inspection fail-PBBT pass (F-P) inconsistency occurred 2.71% of the time on average. This high correlation (near 70%) shows value in using a PBBT as an enforcement tool. It is evident that the PBBT machine picks up on specific wheel-ends incurring a violation seen in the P-F wheel-end statistics. This feature can allow for possible diagnosis of failed brake hoses or other internal air system components. Finally, the F-P scenario suggests that there are certain instances in which the PBBT cannot mechanically find a fault, indicating that there will still be a need for officers to visually inspect vehicles.

Ensuring the Coplanarity of Tiled Optical Surfaces

Michael Dawson-Haggerty (TUFTS UNIVERSITY, MEDFORD, MA 02155), **Paul O'Connor** (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). The Large Synoptic Survey Telescope (LSST) is a proposed ground-based telescope that would have a uniquely large field of view, allowing it to image a large section of sky. This introduces numerous engineering challenges, one of which, addressed in this project, is the coplanarity requirement of the focal plane, a peak to valley requirement of 6.5 microns. The surface consists of a mosaic of imaging chips divided onto "rafts", 120-centimeter square packages each holding nine chips. Each chip is mounted at three points with a sixty micron per turn differential screw at each one. These mounting points allow the surface of the sensors to be adjusted with a resolution of less than one micron by combining instant position feedback from a 0.1 micron resolution confocal laser displacement sensor and precise threads. To bring the surface to flatness, the displacement sensor was positioned over the mounted tiles by a gantry system, and the value was read. To eliminate

the mechanical error from the gantry, we then repeated the scan on a control surface, a commercial optical flat with a specified coplanarity of several wavelengths of light, and subtracted the control surface from the data. There was a significant amount of drift in the gantry due to temperature, but we were able to bypass this by scanning fewer points. We then mapped a plane to each sensor, and used the average plane to calculate the adjustment for each differential screw. By repeating this process we were able to bring the average planes flat to 1.8 microns and total peak to valley flatness to under 6.5 microns. While we were able to bring the surface to the required flatness, there are concerns about the stability of the positioning once the raft is cooled to its operating temperature. Further study and extensive stability testing will be required to ensure that the final focal plane meets all specifications.

Greenhouse Gas Emissions Life Cycle Assessment and Carbon Payback Times for Parabolic Trough Concentrating Solar Power Storage Systems

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Concentrating solar power (CSP) systems have the potential to provide the world with clean, renewable, cost-competitive power on a large scale. CSP plants emit virtually no greenhouse gases during operation because they utilize solar energy and do not burn any fossil fuel. One key advantage of CSP plants over other renewable technologies is their ability to store energy and produce electricity during the period of highest power demand, thus helping to meet the utility's peak demand. This study determines how much carbon will be emitted for two CSP storage systems and how long it will take for each system to "payback" the energy that was consumed, or emissions that were caused, during the systems' entire life cycle. The plant studied in this project is a hypothetical 100-MW parabolic trough plant located in the southwest United States. Upon completion of a thorough materials list, to determine a carbon footprint for a system, several life cycle inventory (LCI) databases and programs were used to track the greenhouse gas emissions associated with the material. In most cases, the output from the LCI program includes the emissions to the air, water and soil due to all the steps of production, including varying levels of transportation. In the LCI discussed in this paper, the focus is on greenhouse gas emissions to the air from the materials included in the thermal energy storage system. Two LCIs were performed and compared in order to determine which storage system has a lesser carbon footprint over its life cycle. This study has shown that the development of a two-tank indirect storage system emits approximately 90 million kg of carbon over its lifetime while that of a thermocline storage system emits 29.4 million kg of carbon over its lifetime. This equates to a carbon payback time of 3.5 years for the two-tank system and 1.1 years for the thermocline system. Since the thermocline system would reduce total costs and carbon, those involved with the completion of the CSP plants currently in development should consider accelerating the development of the thermocline system in order to employ it for CSP plants as soon as possible. Since the molten salt is the system's largest contributing material to climate change, it would be helpful to research other fluids and salts in order to develop a storage medium with a lesser carbon footprint, resulting in a reduced total carbon footprint.

* Performance Prediction of a Solar Thermal Collector Array

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The aim of this summer's project was to predict the performance of a solar collector array that will be part of a prototype solar thermal combisystem. A solar combisystem is a revolutionary system that uses both solar and non-solar energy to provide heat and hot water to a building. The demo system, to be installed in the next 12 to 24 months, will be used to supply part of the heating and domestic hot water demand of Building 30 on the Brookhaven National Laboratory (BNL) campus. The solar array will consist of five collectors covering a total area of 13.70 m². Various resources were used during the course of the project. An extensive bibliography provided valuable knowledge about the factors influencing the performance of a solar collector. Simulation software such as Volker Quaschnig's "Sun Position Calculator" was used to confirm some calculated data. Typical Meteorological Year (TMY) data sets were utilized to find local meteorological information. The final results were computed by using Microsoft® Excel and Visual Basic Editor to combine TMY records with the collector efficiency calculations. The five panel solar array under consideration for installation at BNL should produce over 32 million BTUs per year and save a total of 231 gallons of oil. The predicted energy outputs will be compared to data gathered from the solar array after its installation. If

the estimates are accurate, the Excel files will be used in the planning of future solar thermal projects.

Simulation of Hydrogen Occurrence in Parabolic Trough Power Plants

Douglas Devoto (UNIVERSITY OF DELAWARE, NEWARK, DE 19716), **Greg Glatzmaier** (NATIONAL RENEWABLE ENERGY LABORATORY, GOLDEN, CO 89401). Hydrogen occurrence in the annulus of heat collection element (HCE) receiver tubes reduces thermal performance of HCEs and decreases overall efficiency of trough solar thermal power plants. Degradation reactions in the heat transfer fluid (HTF) used in power plants, most commonly Therminol™ VP-1, produce hydrogen as a byproduct. Hydrogen is distributed through all parts of the plant where the HTF is present and eventually permeates through piping and equipment to ambient air. Hydrogen permeating through HCE receiver tube walls forms an equilibrium partial pressure in the annulus region and causes increases in thermal losses. This report describes the development and preliminary results of a hydrogen model created in Engineering Equation Solver (EES). The model simulates the hydrogen generation and permeation processes to predict the annulus pressure developed in HCEs. It also evaluates several solutions to minimize hydrogen pressure in annuli of HCEs. Combining solutions of relocating a trough plant's expansion vessel directly before the solar array, including a permeation barrier coating on HCEs, and adding hydrogen venting would help to reduce the annular partial pressure in HCEs from original levels of 0.9 to 1.0 torr to acceptable levels of 0.001 to 0.004 torr.

Noise Characterization of the SIDECAR ASIC Readout Chip

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The System for Image Digitization Enhancement, Control and Retrieval (SIDECAR) Application Specific Integrated Circuit (ASIC) is intended for use in the Supernova/Acceleration Probe (SNAP) to provide some understanding of the accelerating expansion of the universe. This single chip serves as an alternative to previous discrete electronics in order to minimize space, weight and power consumption. With the ability to provide a pure digital interface for operating an infrared array and to operate under cryogenic temperatures down to 30K, the SIDECAR ASIC is ideal for all aspects of imaging array operation and output digitization. The primary objective of this work is to measure the variation of noise within the SIDECAR as a function of various key parameters. Optimal noise performance is required for the successful implementation of the SIDECAR ASIC. To achieve this, a test procedure has been developed to measure the noise in each captured image by taking several images after each modification of the microcode and comparing corresponding pixels. The test results show that adjustments to the pre-amplifier microcode configuration have the greatest effect on the noise level. Through such microcode modification, the noise level of the SIDECAR has been reduced by a factor of two, thus approaching the optimal level for implementing the SIDECAR. Future work will focus on testing the SIDECAR ASIC under cryogenic temperatures, as well as in conjunction with the Hybrid Visible Silicon Imager (HyViSI) imaging sensor.

Technology Forecast for Broadband Communication

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We looked at current communication technology and forecast the evolution of broadband communication networks as they become more efficient, more resilient and more robust. Our study places special attention on a competent solution to post-disaster communication barriers currently faced by first responders in the United States. We reviewed 15 wireless broadband deployments, referenced 20 journal articles, tracked broadband communication news articles dating back seven years, and referenced the white pages of fixed and wireless technology providers to develop an informative prediction on the leading broadband communication technology. Our findings show that IEEE Standard 802.16e-2005 is the next innovation to facilitate a broadband communication network that is more efficient, more resilient and more robust than that which is currently in operation. Worldwide Interoperability for Microwave Access (WiMAX), the trade name for this IEEE open standard, provides "last-mile, best-effort" broadband data transmission to send up to 30 megabits of data per second (Mbps) to residential customers and small businesses. In contrast, proprietary transmission rates are up to 6 Mbps for Digital Subscriber Lines (DSL), and up to 12 Mbps for coaxial cable. WiMAX is a robust and resilient Internet Protocol (IP) based data transmission platform using smart Multiple Input, Multiple Output (MIMO) antennas with beam forming in a mesh network configuration along with Orthogonal Frequency Division

Multiplexing (OFDM) to transmit data over 4.82 kilometers; IEEE 802.11 Wireless Fidelity (Wi-Fi) has only 100-meter transmission. The WiMAX base stations (BS) can ideally be used as an internet backhaul to securely transmit data 14.48 kilometers in a non-line-of-sight (NLOS) environment and 48.28 kilometers in the line-of-sight (LOS). These innovations present WiMAX as a justifiable option for communication in areas where data network infrastructure is minimal or non-existent, thus providing cost effective broadband data transmission in rural areas. We suggest ongoing evaluation of WiMAX deployments to determine the best use by region in the United States with regard to disaster response and rural deployment. The WiMAX standard's ability to create more efficient, more robust and more resilient communication systems thus limiting the amount of lives lost in times of peril due to lack of interoperability demonstrates the value of this research to the global community.

Characterization of Nano-Sized Hydrodesulfurization Catalyst Derived from Metal Carbonyls by Sonication

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The strict environmental regulations to limit sulfur to <20 ppm in refined fuels are a new challenge facing refineries. Sulfur removal is crucial not only because of adverse effects of sulfur compounds (SO_x) on the environment, but also because it prevents catalyst deactivation during refining processes. Previously developed techniques such as adsorption, alkylation, extraction and hydro-desulfurization (HDS) conditions do not perform well over residual sulfur in the presence of polyaromatic sulfide derivatives. It is known that the refractory compounds such as dibenzothiophene (DBT) derivatives are desulfurized with nano-catalysts. Molybdenum disulfide (MoS₂), a nano-catalyst, is suspected to be an effective hydro-desulfurizing agent. In order to investigate the HDS properties of MoS₂ as well as to explore the sonolysis as a feasible MoS₂ synthesis technique, we embarked on a project where an unsupported nano-phase MoS₂ HDS catalyst was synthesized in hexadecane by sonolysis of a metal carbonyl (Mo(CO)₆) at -50 °C for 35 hours. The resultant MoS₂ was characterized for particle size, shape and crystalline structure using Scanning Electron Microscopy, X-ray Diffraction (XRD), Energy Dispersive X-ray Spectroscopy (EDAX) and Computed Microtomography (CMT) techniques. The resultant product of Mo(CO)₆ and S in 1:2.5 and 1:5 molar ratio has a cluster-like nature where the individual particles are not distinguishable. The EDAX elemental analysis of both products confirmed the presence of Mo, S, C and O in variable concentrations. The XRD pattern of the product showed a broad peak at 2θ=40° which may be a combination of peaks at 2θ=32.7° and 39.5° which are assigned to the (100) and (103) lattice planes of MoS₂ respectively. Moreover, another broad peak at 2θ=58° corresponding to (110) and CMT 2-D and 3-D images confirmed the presence of nano-sized particles and the absence of MoS₂ crystallites with high defect densities. The experiment demonstrated sonolysis to be a feasible nano-MoS₂ synthesis technique with >90% yield of the desired nano-MoS₂.

Heavy Truck Duty Cycle Data Collection

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Real-world data on Class-8 truck operation is necessary for fuel efficiency studies as well as for use in vehicle powertrain design software. To gather this data, six Class-8 trucks were instrumented with a data acquisition system (DAS) and a set of sensors to monitor numerous vehicle performance parameters from engine to tires, as well as weather conditions, road slope and load weight over a one year period. First, each truck's J1939 vehicle network was tested to learn what vehicle performance information was available on it, and how to retrieve the data of interest. The other sensors and DAS were then installed on each truck, and all data was recorded to the DAS as the trucks then continued in regular operation. During operation, data was checked weekly for errors to determine whether the equipment was functioning correctly. By checking the data, it was discovered that weather sensors began failing from water entry due to unexpected pressure washing of the trucks. Load weight data was found to be inaccurate, as truck drivers had not correctly calibrated the weighing system. Road slope and vehicle network data results were as expected. It was concluded that weather sensors should be covered during pressure washing, and an alternative method for calibrating the weighing system was devised. It was also concluded that the method used to obtain road slope, a derivation from GPS vertical and ground velocity data, was adequate. Finally, it was determined that no changes needed to be made in the method of communication with the

vehicle network. Data will continue to be checked for errors throughout the remainder of the one year test, and corrections will be made as necessary.

Determining the Ability to Monitor the Viability of Transplant Rat Glioma Cells with an Optically Enhanced Catheter

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Approximately fifty thousand cases of Parkinson's Disease are diagnosed within the United States each year. This debilitating disease results from the dissolution of dopamine-dependent communication between the substantia nigra and the striatum of the brain. Cellular replacement therapy, in which stem cells are introduced to supplant dead or stressed cells, has shown promise in animal models. However, the viability of transplanted cells and their survival rate is poorly accounted for by early tests. A novel design coupling a surgical catheter with fiber optic technology provides a tissue delivery platform that can monitor cell viability with sensing techniques widely accepted in the medical industry. The goal of this work is to monitor the health of transplant cells in real time at the final point of delivery using the optically enhanced catheter. Rat glioma cells were separately labeled with CellTracker Orange (CTO) (Invitrogen) and JC-1 stain from BioVision's MitoCapture Mitochondrial Apoptosis Detection Kit and fluorescence was characterized by confocal microscopy. CTO exhibited a single emission peak at 570 nm upon excitation with a 488 nm argon laser. JC-1 exhibited two emission peaks corresponding to fluorescence of viable cells and apoptotic cells, 595 and 540 nm respectively. JC-1 was used to monitor the viability of cells under apoptotic conditions induced by incubating JC-1-labeled cells with carbonyl cyanide 3-chlorophenylhydrazone or etoposide. Observation of fluorescence using a mercury fluorescence microscope over a four hour period demonstrated JC-1's ability to shift in color to reflect cell viability. To detect cell movement through the catheter, cells were labeled with CTO, excited by an argon ion laser with a 501 nm wavelength and a peak emission at 570 nm was detected by an Ocean Optics spectrometer. JC-1 was also used to detect the movement and the viability of cells through the catheter. Cells excited by an argon ion laser with a 488 nm wavelength exhibited emission peaks at 540 and 595 nm, demonstrating the ability to detect both viable and apoptotic cells at the final point of delivery. From the detection of rat glioma cells labeled with CTO and JC-1 using the diagnostic catheter, and the characterized response of JC-1-labeled cells to apoptotic conditions, it can be concluded that these fluorescent probes are suitable for tracking and monitoring the viability of transplant cells through the optically enhanced catheter.

Explaining Leakage in HTS Wires and Cables

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Bi-2212 superconducting wire has a much higher critical temperature and critical current than NbTi, making it a promising replacement material for the construction of high field accelerator magnets. Bi-2212 powder filaments are placed in a silver matrix within silver wires. These wires are then wound into cables and heat treated at 890 °C in a pure oxygen environment to allow powder grains to sinter together. When these cables are covered in insulation, Bi-2212 is observed to leak through the casing during heat treatment. Possible reasons for leakage include cracks in wires, diffusion of Bi-2212 through the matrix, and cracks created in the winding process. This project tested all three of these possibilities. Chemical penetrants were applied to new wires to detect possible cracks. A scanning electron microscope (SEM) was used to search for cracks in both green and heat treated wires. SEM was also used to examine cross sections of wires in order to find Bi-2212 constituents outside filaments, which would indicate diffusion through the silver matrix. Slurries made from oxide powders were applied to the surface of wires. Slurries were also applied to the edges of cables to find out if the cable winding process increases the chances of leakage. The wires and cables were then heat treated and leakage was observed with both an optical microscope and a SEM. Penetrant tests and SEM examination revealed no signs of cracks on green wires. SEM examination of the surface of heat treated wires found no Bi-2212 constituents. SEM examination of wire cross sections found a ring of Bi-2212 constituents between the outer casing of the wire and the silver matrix. This indicates that intense heat treatments may cause a void between the casing and the silver supported matrix, which might stimulate leakage. The slurry tests discovered leakage on some of the wire samples and one of the cable samples, indicating leakage during heat treatment. Leakage observed in cable samples was much greater,

implying that the cable winding process exacerbates, but does not cause leakage.

Noninvasive Optical Detection of Retinal Neurotransmitters and Metabolic Coenzymes

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Changes in physiological concentrations of the metabolic coenzymes nicotinamide adenine dinucleotide (NADH) and flavin adenine dinucleotide (FAD) and of neurotransmitters such as glutamate can be indicative of a number of different disease states. For example, an increase in the ratio of NADH to FAD in a given tissue signifies a decreased rate of aerobic cellular respiration, an indicator of decreased tissue viability for transplanted organs. Also, increases in the concentration of the retinal neurotransmitter glutamate in the vitreous humor have been linked to glaucoma, an ocular disorder that is one of the leading causes of blindness in the United States. Current in vivo detection methods for these molecules are invasive, indirect, or time-delayed. Research was conducted to explore the use of noninvasive optical methods to detect NADH and five of the major neurotransmitters of the retina: glutamate, glycine, gamma-aminobutyric acid (GABA), serotonin and dopamine. Solutions of NADH were examined by ultraviolet-to-visible (UV-Vis) absorption spectroscopy and fluorescence spectroscopy. Additionally, solutions of glutamate, glycine, GABA, serotonin and dopamine were analyzed by UV-Vis absorption and Raman spectroscopies. Varying concentrations of the analytes were used to determine the lowest detectable concentrations, and spectra were analyzed to find distinctive characteristics to enable identification of individual analytes in a complex biological matrix. Porcine ocular fluid samples were collected and analyzed ex vivo using Raman spectroscopy to check for identifiability of the individual species. Fluorescence spectroscopy results indicated that NADH fluoresces detectably with a peak emission at 495 nm when using 405 nm excitation. No other molecule studied was found to have unique absorptions or emissions in the visible range. Distinctive Raman signatures were obtained in vitro for glutamate, GABA and glycine, and glutamate was determined to be detectable at 0.5 M concentration. No analytes were detectable in ocular fluid samples ex vivo. These results indicate that fluorescence and Raman spectroscopy can be used to detect NADH and retinal neurotransmitters, respectively, in vitro and that these techniques may have potential for detecting these molecules in vivo. Future work will be directed to measuring these analytes in ex vivo biological samples by developing a system with sufficient sensitivity to detect physiological concentrations.

*** Design of a 1 kW Proton Exchange Membrane (PEM) Fuel Cell with Dual Cooling Systems**

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Across the United States, the growing recognition of hydrogen's potential as a fuel has increased hydrogen research and development. The theoretical efficiency of fuel cells is higher than that of the internal combustion engine which represents the main source of energy for today's transportation vehicles. In a Proton Exchange Membrane (PEM) fuel cell, the power output is influenced by the humidity and temperature inside the power stack. The electrochemical reaction inside a fuel cell produces 50% energy in electric current and 50 percent energy in heat. Therefore, a cooling system must be designed as a part of the power stack in order for the fuel cell to function safely, not exceed 80 °C, and maintain the Membrane Electrode Assembly (MEA) in a good working condition. In this project, various cooling systems have been designed, utilizing Inventor CAD software, to absorb this excess heat and maintain the fuel cell operating at a safe temperature level. Each design was transferred seamlessly to Finite Element Analysis (FEA) software (Algor) to perform heat transfer and cooling analysis which determined the optimum cooling system and the entire power stack configuration. Dual air cooling systems using fins and air flow conduits were shown to be the best method with minimal parasitic power necessary to operate a cooling fan, unlike liquid coolant which would require more parasitic power from the fuel cell and produce lower efficiency. FEA shows that the finned design cools 10 degrees more than using conduits alone. The FEA also tells us how much air flow is needed through the conduits in order to keep the stack under 80 °C. The final stage of this project was to optimize the design of the power stack so that it contained an optimal number of cooling plates. The fixed cost and the running cost were compared and showed that the running cost of a cooling fan was almost negligible. With this information, the 1 kW fuel cell can be optimally cooled.

Sidearm: Detection and Communication of Events to the Automated Weapon Inventory System

Jesse Fritz (TENNESSEE TECHNOLOGICAL UNIVERSITY, COOKEVILLE, TN 38505), James Younkun (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). A microprocessor based device was designed, implemented and tested for the detection and communication of events to the Automated Weapon Inventory System (AWIS). AWIS is a weapon and related asset tracking system which uses low-frequency radio tags. The device designed, called a Sidearm, detects events such as motion, light beam breaks, or pressure pad activation, and sends a message to the AWIS server, which then initiates a scan and updates inventory status. The Sidearm's purpose is to provide flexible event notification to the AWIS system. This device is of extreme importance to the AWIS system as it is responsible for detecting environmental events that cause the system to scan for inventory changes. The development of Sidearm was made possible by the Rabbit Semiconductor RCM 4200 core module. This device has the ability to serve web pages, link equipment to the internet and control remote devices. In addition, Dynamic C programming software was used to write Sidearm's firmware. An Oak Ridge National Laboratory custom printed circuit board utilizes the RCM 4200 and firmware to create the Sidearm package. The Sidearm program code runs on the RCM 4200 and performs event detection and transmission. The device also features a web-based graphical user interface (GUI) for user configuration. The GUI displays and provides the ability to configure the AWIS server internet protocol (IP) address, the Sidearm's IP address and a time delay filter variable used in the processing of event triggers. The program's GUI uses rigorous error checking functions. Errors are immediately reported, and only valid entries are accepted from the user. The web-based GUI provides the ability to change variable values easily so that the device can be configured for different operating parameters without requiring special tools or knowledge.

Effect of Chemistry on the Life and Performance of High-Power Lithium-Ion Cells

Magdalena Furczon (UNIVERSITY OF ILLINOIS, CHICAGO, CHICAGO, IL 60680), Daniel Abraham (AMES LABORATORY, AMES, IA 50011). High-power battery technology is key to the commercial success of hybrid electric vehicles (HEVs). These vehicles combine the advantages of the extended driving range and rapid refuelling capability of a conventional vehicle with the increased fuel economy and reduced exhaust gases of an electric vehicle. The relatively high specific-energy and specific-power characteristics of rechargeable lithium-ion batteries make them an attractive alternative to the nickel metal-hydride batteries used in hybrid vehicles currently on the market. The goal of this project is to determine the suitability of various electrode-electrolyte combinations for HEV applications. The cells typically contain a layered oxide-based positive electrode, a graphite-based negative electrode and an electrolyte containing an organic solvent and lithium-bearing salts (such as LiPF_6). Project activities to date have involved investigation of the effect of alternative salts, such as $\text{LiF}_2\text{B}(\text{C}_2\text{O}_4)$ and $\text{LiB}(\text{C}_2\text{O}_4)_2$, on cell cycling performance. Experiments were conducted on ~2 mAh coin cells and on ~35 mAh cells containing a lithium-tin reference electrode. The cells were electrochemically cycled or subjected to above-ambient temperatures (up to 55 °C). Capacity and impedance measurements were made periodically to determine the deterioration of cell performance with age. Initial data indicate that cells containing the $\text{LiF}_2\text{B}(\text{C}_2\text{O}_4)$ salt show better long-term performance than do cells containing the LiPF_6 and $\text{LiB}(\text{C}_2\text{O}_4)_2$ salts.

Engineering an Affordable and Handheld Nucleic Acid Dipstick System Prototype for Rapid Field Pathogen Detection

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The development of an inexpensive, reliable, user-friendly and self-contained molecular diagnostic assay is needed for diagnosis of present and emerging infectious diseases in resource-limited settings, and high-throughput disease screening in developed countries. To facilitate the necessary bio-chemical reactions, an effective and embedded heater and micro-fluidic dispensing and flow control mechanism must be engineered and controlled by a microprocessor. In effectively engineering the prototype of this device, the heater was designed and located to promote efficient heat transfer to the solution. The liquid dispensing device uses a nickel-chromium alloy heating element to sear open a pressurized capsule. The subsequent pressure equalization in the dispenser expels the liquid that was held in by capillary forces. The micro-fluidic flow control mechanism uses a shape memory alloy as an actuator to regulate flow. A microprocessor electronically controls the heater and the micro-fluidic dispensing and control mechanisms,

thus permitting an autonomous system. Each of the above individual components has been modeled and demonstrated successfully. The next step is to assemble them into a functional Dipstick prototype. This prototype will then serve as a model for the final design stage prior to manufacturing. An effectively engineered system will allow the Dipstick to perform at its full potential. Such a design has the potential to revolutionize clinical diagnostics, and afford improved health care to people throughout the world.

Thermal Investigation and Management of a Polymer Electrolyte Membrane Fuel Cell Stack

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Thermal management systems designed to control temperature and humidity inside a Polymer Electrolyte Membrane (PEM) fuel cell are crucial to optimizing its performance and efficiency since temperatures within the fuel cell that are higher than 80 °C reduce the efficiency of its electrochemical process by increasing the membrane's malleability and escalating the permeability of reactant gases. Accordingly, to aid in the design of a thermal management system for a PEM fuel cell, an experimental setup was built to observe the internal temperature of a fuel cell power stack during normal operating conditions and under variable power loading levels. A ten-cell power stack with three plates at the beginning, middle and end — each fitted with five thermocouples — was used to monitor the internal temperature of the stack. Tests were run, each at a different humidity above and below 30 °C, because the humidity requirements of the stack change with temperature. During each test the current of the electrical load was gradually increased while all humidity levels, power outputs and stack temperatures were monitored and recorded. When the heat and electrical power produced was graphed against time, it was seen that both increased at about the same rate, proving that the ratio of heat to electrical power was about 1:1. Therefore, with higher cooling loads expected at higher currents more parasitic energy is also required to cool down the fuel cell stack. Thus, it is recommended to run the fuel cell stack at lower currents to increase the efficiency and minimize the parasitic energy necessary to operate its cooling systems.

The Hybrid Cu-Cl Thermochemical Cycle: Crystallization and Hydrolysis of CuCl_2

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One of the more promising methods for producing hydrogen is the hybrid copper-chlorine (Cu-Cl) thermochemical cycle. One of the main attractions of the hybrid Cu-Cl cycle is that it requires a relatively low temperature heat source compared to other thermochemical cycles. The crystallization and hydrolysis of CuCl_2 are two key steps in the cycle. The hydrolysis of CuCl_2 is a reaction with water which forms Cu_2OCl_2 and HCl at 400 °C. One of the main problems with this reaction is the need for excess water, and a competing decomposition reaction which forms $\text{CuCl}(\text{s})$ and $\text{Cl}_2(\text{g})$. The operational parameters for a continuous spray-type hydrolysis reactor were studied and optimized by analyzing the composition of the solid products obtained via X-ray diffraction techniques. Overall, tests have shown that reactor temperatures at or above 400 °C tend to favor the formation of CuCl and that increasing the residence time of the copper (II) chloride solution is essential for achieving complete conversion of CuCl_2 . Another step in the cycle's process design, the crystallization of CuCl_2 , was also studied. Data were also collected and compared to literature data for the solubility of CuCl and CuCl_2 in water at various concentrations of HCl . This effort was carried out at room temperature for CuCl , and at 10, 25 and 55 °C for CuCl_2 . Although all data collected for the solubility of CuCl_2 agreed with the available literature, the data obtained for the solubility of CuCl remains inconclusive. Higher temperatures favor the decomposition reaction (formation of CuCl) and a longer residence time improves the fractional conversion of CuCl_2 drastically. Analysis of the data suggest that increasing the temperature of either the reactor or the superheated steam entering the reactor increases the amount of copper (I) chloride formed. Because the goal of this experiment was to minimize the formation of CuCl and ultimately obtain a nearly pure copper oxychloride product, this result is essential to the successful hydrolysis of copper chloride. From the results, it is clear that a furnace temperature of 370 °C should give a minimal amount of CuCl and unreacted CuCl_2 , while still forming enough Cu_2OCl_2 .

Superluminal RF

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A source of electromagnetic radiation is said to be superluminal when

its velocity exceeds that of its emitted waves ($v > c$) *in vacuo*. This allows for superluminal sources to make multiple contributions to the electromagnetic field of an observer at some point. In particular, pulsar emissions have been demonstrated to result from modulated waves formed by superluminal distribution patterns of the polarization current rotating within a pulsar's plasma atmosphere. Radiation from a rotating superluminal source forms a cusp, where waves emitted over a long period of source time are received simultaneously by an observer on the cusp. The power emitted by the cusp decays as a function of the inverse radius from the source ($1/R$, rather than the conventional inverse square law), presenting unique potential for applications in radar and directed-energy technologies, secure communications and astrophysics. To simulate this phenomenon experimentally, a specialized circular antenna was designed, composed of 72 individual antenna elements, each receiving a different modulated signal input. By varying the phase relationship between these signals, the angular velocity around the antenna multiplied by the antenna's radius, results in a $v > c$. Phase one of the project involved determining the most effective method of achieving signal modulation with full amplitude and 360 degrees of phase control using ADL5390 vector multipliers. To complete the preliminary portion of the project, a control system was designed to specify amplitude and phase in an 8 channel prototype of the eventual 72 channel system. Implemented with LabVIEW code, the control system is capable of setting the signal to an accuracy of within 0.5 dB of the desired amplitude and one degree of the desired phase.

Sewage Treatment Plant Optimization for Reduction of Nitrates

Alexander Hoimes (PENNSYLVANIA STATE UNIVERSITY, UNIVERSITY PARK, PA 16801), Robert Lee (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Sanitary and process wastewater generated by Brookhaven National Laboratory (BNL) operations is conveyed to the Sewage Treatment Plant (STP) for processing before discharge to the Peconic River. Under a permit issued by New York State Department of Environmental Conservation (NYSDEC), the STP uses a discharge point authorized under the State Pollutant Discharge Elimination System (SPDES) which regulates wastewater effluent at the laboratory. Starting in February 2005, the STP effluent total nitrogen concentrations began to exceed the SPDES limit of 10 mg/L. As a result, BNL has been investigating the potential sources of elevated nitrogen concentrations observed at the STP. Lower than normal flow conditions and decreased nutrients in the waste have been identified as the most likely causes to the increased levels of nitrogen in the discharge. This research evaluated and determined the correlation between dissolved oxygen, total nitrate and nutrient loading at the STP. With this information, the STP process can be optimized to minimize the release of nitrogen into the Peconic River. Using commercially available test equipment, the levels of nitrate (the predominant component of the STP total nitrogen measurements) and dissolved oxygen were measured during the STP treatment sequence. The concentrations were tracked and plotted during periods of supplemental nutrient addition to the STP and during periods of sustained nutrient addition. Rates of nutrient addition were also measured daily and compared to base load nutrients in the STP influent. Nutrient loads were measured using contract analytical laboratory analysis for Biochemical oxygen demand (BOD), and based upon a 24-hour composite sample. From this, we concluded that the addition of nutrients to the STP is a necessary ingredient to keeping the nitrate levels from exceeding the SPDES limit.

Formation and Dissociation of Methane Hydrates in Consolidated Sand: Duplicating Methane Hydrate Dynamics beneath the Seafloor

Kristine Horvat (STATE UNIVERSITY OF NEW YORK—STONY BROOK, STONY BROOK, NY 11794), Devinder Mahajan (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

Methane hydrates, inclusion compounds where water molecules form an icy cage to surround a methane molecule, occur in permafrost and marine environments where high pressure and low temperature conditions coexist. Estimates of more methane in nature in the form of hydrates throughout world than any other fossil fuel have sparked an interest in hydrates for a potential energy supply for decades. However, there has been growing evidence that methane hydrates play a crucial role in seafloor stability and global warming. To alleviate these problems, more must be understood about sediment-hydrate interaction during dissociation. In this study conditions under the seafloor have been duplicated in the Flexible Integrated Study of Hydrates (FISH) Unit to observe the pressure, temperature and gas output responses upon methane hydrate formation and dissociation. The FISH Unit consists of a pressurized Temco cell filled with water saturated Ottawa sand maintained at a low temperature and high pressure. After charging methane gas, methane hydrate formation pressure-temperature

(PT) kinetics are monitored over time until pore pressure reaches an asymptote at hydrate equilibrium pressure. Dissociation is achieved through depressurization from equilibrium predictions in pure water and pure methane, and cooling due to the endothermic nature of hydrate dissociation is observed throughout the sample using thermocouples placed at different lateral and radial positions. During dissociation, temperature monitoring shows that the center radius of the cell drops in temperature more rapidly than the middle radius, thereby indicating that hydrates start to dissociate from the center of sample towards the walls. In addition, calculations using PT data collected shows that the enthalpy of dissociation is found to be 59.45 kJ/mol, which confirms previously reported calculations of 56.43 kJ/mol. Also, post-depressurization PT equilibrium fit theoretical data for methane hydrates; therefore methane hydrates were indeed formed.

Distributed Energy Communications and Control Laboratory Enhancement

Philip Irminger (UNIVERSITY OF TENNESSEE—KNOXVILLE, KNOXVILLE, TN 37996), John Kueck (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). The Distributed Energy Communications and Control laboratory (DECC) is a one of a kind research facility at Oak Ridge National Laboratory (ORNL). The DECC is used for testing the operation of inverter-based and generator-based Distributed Energy (DE) resources interfaced with the electric power system to provide reliability services. The reliability service we are studying now is rapid, local voltage regulation. The DECC lab is unique because it is interfaced with an actual distribution system — the ORNL central campus distribution system. The objective of my work was to help identify instrumentation and control requirements for a large inverter at a location remote from the main DECC Lab. The DECC Lab currently has one inverter-based DE test system that was used to establish the baseline for rapid inverter voltage control methods. Since the new large inverter is remote from the main laboratory and involves remote operation, many of the controls had to be modified. An off-the-shelf automated logic system was found to be the best solution in terms of flexibility and compatibility for controlling and monitoring the new inverter system. The instrumentation and control requirements were determined and specifications were provided for the ordering of the new control hardware. The next step will be to determine the best physical and electrical configuration for the remote inverter test system. After the installation is complete, we will test the control capabilities offered by the automated control system. The DECC lab at ORNL is continually exploring new ways to make the electric grid more reliable and robust using reliability services from DE.

Effects of Friction Stir Processing on Scuffing Resistance, Friction and Wear Performance and Hardness of Bronze

John Jast (UNIVERSITY OF ILLINOIS, URBANA-CHAMPAIGN, URBANA, IL 61801), Cinta Lorenzo-Martin and Oyelayo Ajayi (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439).

Friction stir processing (FSP) is a surface-engineering technology used to locally modify a material's microstructure and eliminate casting defects to enhance specific properties. FSP often results in increased resistance to corrosion, improved strength and hardness and enhanced formability. The technology involves a rapidly rotating tool with a small diameter pin (6 mm) and larger diameter (16 mm) concentric shoulder being plunged into a surface (a few mm) and traversed along the surface in the direction of interest. The friction created between the tool and the workpiece creates heat and results in metal deformation (modifying grain size) but not melting. This frictional heating and extreme deformation causes the plasticized material to flow around the tool and merge behind it. Overall, the process creates a finer, homogeneous microstructure with equiaxed grains, increases yield and tensile strengths, and virtually eliminates casting defects such as porosity. The objectives of this project were to determine how FSP affects the friction and wear performance of a material, its resistance to scuffing, and its hardness. In order to complete these objectives, base bronze and friction stirred bronze samples were tested using a block-on-ring test rig for friction and wear performance and Vickers tests for quantifying hardness and creating surface hardness profiles. Friction and wear data were compiled and analyzed to determine if a finer grain size due to the FSP resulted in improved friction and wear performance and an increase in scuffing resistance, as expected. In addition, the effect that FSP has on a material's hardness was explored. Data shows that FSP resulted in a 19–33% increase in surface hardness of bronze. In addition, FSP resulted in a 72.8% decrease in wear amount and up to a 58.0% decrease in surface friction coefficient. However, the FSP technology had no significant effect on the resistance of bronze to scuffing. As this investigation continues, the effects of FSP on the friction and wear properties of other materials needs to be explored. In addition, further studies need to be conducted to determine the extent

to which FSP processing parameters, including tool speed and number of tool passes, affect surface hardness, friction and wear performance and scuffing resistance.

*** Imaging Residual Immiscible Fluids at Different Wettability Conditions of Permeable Media**

Maude Johnson, Meagan Pinkney and Lindsey Thomas (SOUTHERN UNIVERSITY AND A&M COLLEGE, BATON ROUGE, LA 70813), Riyadh Al-Raoush and Mark Rivers (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). In this research, microtomography was used to image the residual saturation of the pore-scale distribution of organic immiscible fluid (Soltrol 220) at different wettability conditions. Boron carbide was chosen as the porous media with a grain size of 250 microns to represents natural sand particles. The boron carbide was treated to obtain systems with different fractional wettability. Four levels of wettability were observed in a percentage ratio of water-wet (ww)/oil-wet (ow) porous media: 100% ww/0% ow, 75% ww/25% ow, 50% ww/50% ow and 0% ww/100% ow. A column with an inside diameter of 6.0 mm and a height of 83.5 mm was used to conduct the flow and entrapment of immiscible organic fluid at the residual level. Changing the wettability was obtained by the Bradford and Leij (1997) procedure, adding two percent by volume of octadecyltrichlorosilane (OTS) to ethanol and saturating the boron carbide completely. Doping the boron carbide with OTS allowed there to be contrast between the de-aired water and organic immiscible fluid in the imaging. Results show that the 100% ww/0% ow system contains a minimal amount of residual saturation. This means the Soltrol 220 is located in small porous areas that resemble being trapped between tightly packed areas of the boron carbide, and the 0% ww/100% ow system has the most residual saturation, with the Soltrol 220 largely distributed amongst the large and medium porous areas, and the de-aired water located in smaller porous areas. The research shows that microtomography is an effective and efficient tool to non-destructively create 3-D images of the oil's distribution. For future research, characterization of the pore-scale distribution of the organic fluid including locations, shapes, sizes, interfacial areas, orientations and correlation at different wettability conditions of the porous media will be studied.

Study of Membrane Poisoning by Sulfur Compounds

Ashley Jones (PRAIRIE VIEW A&M UNIVERSITY, PRAIRIE VIEW, TX 77446), Costas Tsouris (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). The objective of this study was to propose a mechanism for Palladium (Pd) poisoning and simulate hydrogen (H_2) flow in simple and composite membranes. We show how mathematical models can be used to describe and predict multiphase separation processes, such as those involving the separation of H_2 from other gases by Pd membranes. This is a theoretical study that includes mathematical derivations and development of computer codes for computations to be performed on a personal computer. Pd alloy membranes have been used to separate H_2 from coal gasification and steam reforming product streams. In many cases, hydrogen sulfide (H_2S) in the process streams deactivates the metal membrane and reduces H_2 permeation and selectivity. H_2 is a very important gas in many industrial fields. Currently, hydrocarbons are the main source for hydrogen H_2 production, and membrane reactors are used to separate the H_2 from other gases that are produced. These reactors combine reaction and separation in the same unit operation. The proposed model predicts H_2 fluxes through composite membranes of several layers for standard operating conditions. The model was constructed for H_2 permeation through Pd and accounts for external mass transfer, surface adsorption and desorption, transitions to and from the bulk metal and diffusion within the metal. The main assumptions in this modeling approach are (i) absence of external mass transfer resistance and (ii) diffusion-limited permeation for pure Pd for temperatures above 573K and membrane thicknesses down to 1 micrometer. Low-temperature permeation of H_2 is limited by desorption, while adsorption is expected to impact permeation only at very low upstream H_2 partial pressures, or under conditions of substantially reduced sticking due to surface contamination. This project deals with ways to design better membranes by developing a model for the poisoning of the membranes by H_2S .

Planetary Gearbox Bearing Calibration for Wind Turbine Gearboxes

Braden Kappius (COLORADO SCHOOL OF MINES, GOLDEN, CO 89401), Hal Link (NATIONAL RENEWABLE ENERGY LABORATORY, GOLDEN, CO 89401). Wind turbine gearbox reliability has been a major concern due to premature failure. The National Renewable Energy Laboratory (NREL) created the industry wide Gearbox Reliability Collaborative (GRC) to better understand gearbox failure mechanisms. One goal of the GRC is to understand how loads and events translate to bearing response,

including reactions, load distribution, displacements, temperature, stress and slip. Computer models predict these responses, but data obtained from real gearboxes is needed to validate these models. By instrumenting gearbox bearings in two gearboxes, one to be field tested and the other to be tested in the National Wind Technology Center's dynamometer, bearing load data can be compared and analyzed. Before the bearings are installed in the gearboxes, baseline load values must be gathered by a bearing calibration method. The bearing calibration applies radial loads ranging from 10 000 to 100 000 lbs to two coaxial bearings mounted on a shaft inside two circular rollers. A model of bearing load distribution provides a relationship between total load and load on each roller. The data collected were used to derive the loading as a single roller element passes. By increasing the load in specific increments and correlating it to the gage response, a direct relationship between the two was determined. The relationship is expressed as: $L_{roller} = A \cdot e_{gage} + B$, where L_{roller} is the roller load in pounds, A is the regression slope (lbs/ue), e_{gage} is the gage response (ue) and B is the regression offset (lbs). The data for each gage is presented in the text. This relationship will be applied to interpret dynamometer and field test data to determine loads on the bearings. Initial results of this research indicated a correlation with the regression coefficient for the roller load equation of greater than 0.98 for the majority of the lines. This high regression coefficient and consistency of coefficients indicate the calibration method to be valid. Future calibration tests could optimize the alignment procedure of the test apparatus and/or to allow for testing of a single bearing at a time.

Implementation of a Proactive Diagnostic Testing Algorithm for Building Automation Systems

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Building automation systems (BASs) have come into widespread use in commercial buildings as computing power has become easily available, communication protocols have become standardized and reliable, and as open control system architectures have driven down the price and commitment necessary to implement them. These systems have the potential to increase building energy efficiency by 15 to 30%. In many cases, improper maintenance causes BASs to operate sub-optimally. Because a BAS can only work efficiently with accurate data, many of these problems are rooted in sensors that need recalibration or replacement. Researchers at Pacific Northwest National Laboratory and Portland Energy Conservation have created an algorithm to automatically detect and diagnose faults in BASs caused by faulty sensors and malfunctioning equipment. This algorithm monitors building conditions through a supervisory control and data acquisition (SCADA) network. If a fault is detected, the BAS initiates tests to isolate the problem and recover from it. A test for diagnosing problems in temperature sensors was implemented with the Python programming language and loaded into an existing SCADA network. This test determines which of three sensors has faulted. Once the faulty sensor is identified, the fault is diagnosed and recalibration or a replacement request is performed based on results. This test operates using only existing sensors coupled with the knowledge that at least one sensor is inaccurate. Automated testing ensures accurate data for systems management, which, in turn, reduces wear and tear on the system, increases occupant comfort and decreases operating expense. This work allows one such test to be performed utilizing existing systems, without the need to purchase additional hardware.

Inkjet Printing of Metal Front Contacts on $Cu(In_{1-x}Ga_x)Se_2$ Thin Film Solar Cells

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Inkjet printing as a manufacturing process is poised to become a viable means of mass producing solar cells at the industrial level. This experiment focuses on optimizing the method of inkjet printing nickel and silver front contacts onto copper-indium-gallium-diselenide (CIGS) thin film solar cells. The proprietary organometallic inks developed by the National Renewable Energy Laboratory (NREL) are deposited using a Fujifilm Dimatix™ Materials Printer retrofitted with a hot plate to allow substrate temperatures of up to 300 °C. Substrate temperature and drop spacing are manipulated to produce uniform, continuous metal lines with a low electrical resistivity. A Transfer Length Method (TLM) test is performed to ensure low electrical contact resistance. Contacts on CIGS cells measuring approximately 0.45 cm² were printed and characterized. The CIGS cells nickel-silver layered contacts were printed, with nickel acting as a barrier to stop silver from diffusing into the solar cell at the elevated printing temperature. The resulting

CIGS cells achieved efficiencies as high as 11.58%, comparable to a reference cell with evaporated contacts. Higher efficiencies are achievable if the printing process can be shortened or the required substrate temperature for ink decomposition can be lowered.

Polysaccharide Accumulation in Nitrogen-Limited Cultures of Two Photosynthetic Microorganisms — *Plectonema boryanum* and *Chlamydomonas reinhardtii*

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Plectonema boryanum and *Chlamydomonas reinhardtii* are two distinct photosynthetic microorganisms that are capable of accumulating polysaccharide storage products (glycogen and starch, respectively) under nitrogen-limited culture conditions. In the presence of light, these high-energy intracellular storage products can be converted by these two microorganisms to hydrogen gas in a process called indirect biophotolysis. Previously published experiments concluded that in cultures of *P. boryanum*, higher production rates of glycogen led to higher subsequent production rates of hydrogen. The purpose of this study was to determine the effects of different culture conditions on the accumulation of these two polysaccharide storage products. Specifically, the effect of dilution rates on glycogen production was studied in continuous cultures of *P. boryanum*, while the production of starch by *C. reinhardtii* was examined using different culturing conditions: batch, fed-batch, semi-continuous and continuous. Both of these microorganisms were grown in continuously agitated and illuminated 1 L Roux bottles sparged with air/CO₂ (99.7%/0.3% vol/vol). For the continuous cultures of *P. boryanum*, a range of dilution rates ($D=F/V$, F =medium feed flow rate, V =culture volume) was tested (0.03, 0.05, 0.13 and 0.20 day⁻¹). It was determined that culture dilution rates between 0.05 and 0.12 day⁻¹ resulted in the highest glycogen productivities in continuous cultures. Moreover, this information complements previous data, confirming that throughout this range of dilution rates, continuous cultures performed less effectively than batch and fed-batch cultures in producing glycogen. The second part of this study was conducted to determine the effects of different culturing conditions on starch productivity in *C. reinhardtii*. The highest starch productivity was observed during the initial growth phase in the batch and fed-batch cultures. Progressively lower productivities were exhibited in the pseudo-steady-state phases of the semi-continuous, fed-batch and continuous cultures.

Enzyme Use in Fuel Cell Applications

Samuel Labarge (RENSSELAER POLYTECHNIC INSTITUTE, TROY, NY 12180), Abhijeet Borole (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Fuel cells are ideal for many applications, but their commercial development has been hindered significantly by problems associated with catalysis. Platinum-catalyzed fuel cells, for example, provide higher power densities than fuel cells catalyzed by other metals. Unfortunately, platinum is expensive and quantities are limited. One alternative to catalysis by platinum is the use of microbes and enzymes purified from microbes and fungi. Most fuel cells catalyzed by enzymes use a planar electrode with alcohols and glucose as the fuel. Our research focuses on developing a three-dimensional enzymatic fuel cell (EFC). We used laccase from *Trametes versicolor* (a polypore mushroom) as the catalyst. This laccase is a copper-centered enzyme that reduces oxygen in air to water. Our device consists of an anode compartment with a platinum-carbon catalyst separated from a cathode compartment. The cathode compartment contains a 1-cm² by 0.5-cm carbon felt that supports an ion-selective Nafion® membrane. The cathode compartment contains a carbon support and a solution of laccase. We attempted to optimize the cathode side of the fuel cell by evaluating its power density in response to variations in concentrations of the enzyme and electron mediator, and differences in the concentration of buffer and solution-loading volume. In response to these variations, we measured fuel cell power densities ranging from 1–12 W/m². While these power densities are still an order of magnitude lower than those of Pt-fuel cells, EFCs have the potential to provide cost-effective mobile power subject to further improvements in power density. Continuing development will characterize and optimize the stability of the enzyme on the carbon support to provide longer lifetimes and higher power outputs.

Analyzing Exhaust Gas Recirculation Contaminated Engine Oil

Andrew Larkin (UNIVERSITY OF ILLINOIS, URBANA-CHAMPAIGN, CHAMPAIGN, IL 61820), Robert Erck (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). Exhaust Gas Recirculation (EGR), is commonly used in diesel engines to reduce emissions of nitrous oxides. However, EGR also contaminates engine oil by adding soot particulates and acidic molecules. The goal of this study was to determine the extent

and mechanism of wear on several different materials using EGR contaminated oils of varying soot content and acidity. The contaminated oils were obtained from a Cummins M11 test with EGR. They had soot percents of 8.4, 10.3, 9.0 and 12.0, with total acid numbers of 1.68, 1.91, 1.91 and 2.36 respectively. The different materials used were 52100 steel, Al₂O₃, ZrO₂ and Si₃N₄. The materials were tested in a Falex four-ball tribological test machine according to the American Society for Testing Materials' protocol, D-4172. The oxides showed very high friction coefficients of about 0.12 while Si₃N₄ was nearly the same as steel at about 0.1. ZrO₂ also showed a strange drop in friction during the tests from about 0.12 to as low as 0.02. This may be due to a phase transition from the high pressures of the rig. It also may have been a false reading caused by the ball's increasing surface area throughout the test which transferred the test into hydrodynamic lift as opposed to boundary lubrication. The balls were then examined for wear using an optical profilometer through interferometry. In these tests, the Si₃N₄ suffered some surface cracking but no measurable material removal while the oxides took above average wear using 52100 steel as a baseline. The wear was determined to be abrasive in nature rather than corrosive. Alumina wore by grain pullout. Si₃N₄ should be retested to determine the maximum loads that it can bear in contaminated oils. The strange friction transition of ZrO₂ should also be probed.

Study of Techniques Used for Demolition of the High Flux Beam Reactor Exhaust Stack at Brookhaven National Laboratory

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The High Flux Beam Reactor (HFBR) stack at Brookhaven National Laboratory (BNL) is a 320 ft structure, still in use by the Hot Laboratory (Building 801), that was once also used to ventilate exhausts from buildings in the HFBR complex and the Brookhaven Graphite Research Reactor (BGRR). The stack is 59 years old and is being evaluated for Decontamination and Decommissioning (D&D). The stack D&D project involves the evaluation of alternative D&D methods, the preparation of technical specifications and detailed project planning which includes implementing work plans and procedures. Due to the stack's close proximity to operating facilities and the internal contamination within the stack itself, the safe methods for removal of the stack are limited. After a study of conventional stack demolition methodologies was performed to select the one most likely to lead to a successful D&D of the stack, rubbleization and segmentation were selected for further investigation. Based on standard elements of environmental restoration projects as discussed in the Environmental Restorations Projects (ERP) department, a set of criteria was created to help choose the most appropriate method for demolition. The criteria used for evaluating the methods included worker safety, costs, scheduling, contamination control and waste transportation and disposal. When using the established criteria to compare the two methods, rubbleization was found to be the more practical approach for removing the stack. Rubbleization is safer than segmentation because the concrete cutting device used to crush the concrete can be remotely operated so that workers will not be operating machinery at elevated heights once the device is in place. Further, crushing and cutting the concrete into small pieces makes packaging and shipping of waste easier and more affordable. Finally, the spread of dust will be minimal due to the application of water spray nozzles to the cutting device. The method of rubbleization was chosen as the demolition technique due to the low safety risks, lower costs and the efficiency of the method. Segmentation was not chosen because of the increased risk due to working at elevated heights, and the troublesome process of size reducing the pieces for disposal. Also, loading and shipping the large pieces increases the risk for potential accidents at the workplace. Budgetary quotes have been acquired from proposed vendors and an approximate work schedule has been created so the length and cost of work are able to be calculated. Funding is not available to begin working on the stack due to the costs of other procedures going on at the BGRR and the HFBR complex. Once funding is available from the Department of Energy, work can begin.

Ergonomics Evaluation of Single Channel Pipettes

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At the Lawrence Berkeley National Laboratory (LBNL) and other science laboratories worldwide, ergonomics is an important issue. Repetitive laboratory activities such as pipetting can cause cumulative trauma disorders (CTDs) for scientists and technicians. The role of ergonomics in a laboratory setting is to assist in the layout of the workplace and design of tools to fit workers and reduce risk factors that can contribute to CTDs. The main purposes of this study were to identify relationships between user characteristics and pipette

preferences and to identify trends in user preferences. The study consisted of 21 users who completed a pipetting task with five manual and five electronic pipettes. Prior to completing the task, each participant completed a brand preference questionnaire to identify their existing biases toward certain pipette brands and models. Their hand length, breadth, strength and digit one (thumb) length were measured. They then filled one 8-well row of a 96-well plate with each pipette, completing three volume changes during the cycle. After filling a row, they completed a rating sheet which utilized a series of visual analog scales (VASS) to rate the pipettes based on a variety of attributes. A Friedman test with a Tukey follow-up was used to determine the statistical significance of the ratings. Although no single pipette was significantly better than all of the others for all of the attributes tested, there were some significant relationships found among pipettes for single attributes. Two sets of rankings were formed using median ratings; the Rainin Pipet-Lite was the dominant manual pipette while the Thermo Finnpiptette Novus was the top ranking electronic pipette. The Finnpiptette surpassed all of the manual pipettes except for the Rainin Pipet-Lite. This is a great advance for electronic pipettes since they provide lower plunger forces and reduced repetition through the use of programs. There was no significant correlation between any measured personal characteristics and ratings of individual pipettes. These results combined with the remarks given by many participants emphasize that the task and setting of use contribute to pipette preferences; although, the significance of rankings suggest that certain pipette features are desirable.

Development of a Supersonic Gas Jet for Ion Beam Diagnostic Purposes

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The research group in the Heavy Ion Fusion Science Virtual National Laboratory (HIFS-VNL) at Lawrence Berkeley National Laboratory (LBNL) plans to increase ion beam intensities for future warm dense matter experiments. Current intercepting ion beam diagnostics are at risk of not withstanding these intense ion beams. Therefore, a supersonic gas jet test stand has been developed for non-intercepting ion beam diagnostic applications. Current research focuses on the first efforts to characterize the supersonic gas jet flow that is generated by a Laval nozzle. The principal objective of the current study is to visually measure the location of the first density knot (Mach disk) that is formed by the self-focusing behavior of an underexpanded supersonic gas flow. The Mach disk will be used as an ion beam target to characterize any ion beam profile in future experiments by measuring the gas excitation by the impinging ion beam. The supersonic gas flow is dependent on the relationship between nozzle inlet pressure, nozzle throat diameter, the vacuum vessel pressure and the gas flow catcher backpressure. The optimal gas catcher-nozzle combination and the nozzle pressure conditions required to generate a slightly underexpanded supersonic gas flow have been investigated. Mach disk locations were recorded with different initial system configuration. Future work will include a redesign of the electrode structures to improve gas flow visualization, the addition of more powerful vacuum pumps to improve the control of the gas jet behavior and the development of experiments to characterize the density profile of the supersonic gas jet stream.

Bridging Dynamic Needs to Solid Engineering

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Facility needs for fuel cell research and development (R&D) are dynamic. Consequently, laboratories will require periodic modifications to meet the demands of this R&D. Current fuel cell prototypes are requiring thousand-hour testing capabilities in which the facilities need to be able to maintain constant control of ambient conditions. This research will require backup power and gas supplies for caustic, explosive, toxic and possibly highly toxic gasses. It has been proposed to modify an existing laboratory building to support the necessities of this long-term testing. The effort starts with a Service Request (SR), the means to initiate any service or facility modification within Pacific Northwest National Laboratory (PNNL). The SR was initiated and submitted by the researchers and building management in order to develop a Project Baseline Document (PBD) which delineates the scope of work, cost and schedule for the proposed facility renovations. Once the SR was received by the Project & Construction Management Group Manager, it was assigned. The Project Manager is responsible for the overall management of the effort which includes the development of the PBD and the coordination needed to gather all the required subject matter experts to obtain the necessary information contained in the PBD and subsequent project phases such as definitive

design, construction management, contracting, safety, etc. As a team we worked together to establish the required functional criteria, recognize and resolve problems and identify risks and their mitigating alternatives. By communicating with the researchers that would occupy this facility, we found that they would need two custom 12 ft x 5 ft fume hoods, with backup generator power for the HVAC systems. Piping leading outside the building will route gasses from gas storage racks to the fume hoods. The PBD will serve as a basis in order for the building manager to formally request the required funds for Fiscal Year 2009, therefore this modification effort will be fully developed and executed next Fiscal Year provided the funds are approved.

Design for Shielding Photomultiplier Tube from External Magnetic Field

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Photomultiplier tubes are used to collect faint traces of light in detectors at Thomas Jefferson National Accelerator Facility. The Photonis XP4508B photomultiplier tube (PMT) will be used to detect light from Cherenkov radiation in the High Threshold Cherenkov Counter in the Continuous Electron Beam Accelerator Facility (CEBAF) Large Acceptance Spectrometer (CLAS). Incident photons strike a photocathode, which emits electrons (via the photoelectric effect) that are gathered and multiplied to produce an electric signal. This process is sensitive to magnetic fields above 0.2 Gauss, and the location of this PMT in the detector will be subject to magnetic fields up to 50 G. The focus of this study was to design a ferromagnetic shielding model to reduce the magnetic field at the location of the photocathode to around 0.2 G in an external field of 30 to 50 G. The program Poisson Superfish was used to model the shielding and external field and to calculate the field strength at the photocathode. A variety of models were tested, varying in number of shield layers (up to three), size and material type. It was found that a three-layer shield comprised of an outer shield of HyPerm49 and inner shields of conetic mu-metal reduced the external magnetic field to the required level for correct operation of the PMT. This result confirms that a three-layer model is necessary to provide adequate shielding from external fields of around 50 G. It also shows that models using regular iron or soft iron will not reduce the external magnetic field to a level low enough to allow the PMT to operate efficiently. For external field strengths up to 50 G, it is clear that the materials HyPerm49 and conetic mu-metal possess superior magnetic properties to provide shielding for PMT's; and the calculations suggest that increasing the number of shields and their thicknesses will further reduce the magnetic field strength.

Medium Truck Duty Cycle Study

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Currently, there exists little knowledge of real-world duty-cycle operations for class-6 and class-7 commercial trucks. The goal of the Medium Truck Duty Cycle (MTDC) project is to provide a comprehensive database that will help improve the efficiency for these classes of vehicles. A data acquisition system (DAS) will be placed on each of six field operational test vehicles to collect the duty cycle information. The data are gathered during normal vehicle operations in order to give more accurate, real-world information about vehicle usage. Each DAS is configured via the internet, using a Raven X wireless modem incorporated in each DAS. Also contained within each DAS is an eDAQ Lite data logger, which performs the data acquisition function. A VBOX II Lite, which logs information such as GPS location, velocity and acceleration, transmits its information to the eDAQ via the J1939 controller area network. Also installed on each test vehicle is an Air-Weigh self-weighing device, which monitors the vehicle's weight throughout the testing period. This information is sent to the eDAQ through the same network as well. A major landmark in the project was the installation of a wireless modem in each DAS. Previously, in a similar project involving class-8, long-haul tractor-trailers, periodic manual travel to the fleet's home base was necessary for on-site data uploads from the DAS units. Through the Raven X modem, the eDAQ webpage is remotely accessible and allows for changes in system and hardware settings. The eDAQ's Test Control Environment Software can be used on a remote computer to view the database information in real-time. The vehicle latitude and longitude information from the VBOX also can be loaded into a mapping program to graphically display the route taken during a specified time. The implementation of the DAS units is not yet complete. After being installed, they will gather duty cycle information for a 12-month period, thus creating a database with seasonal representation. This project provides data that can lead to improvements in the efficiency and safety of class-6 and class-7

commercial vehicles. Future studies could focus on characterizing driving patterns, fuel trends and the effects of geometrics, weather and other factors on vehicle performance.

Developing Genomics-Scale Throughput for Small Angle X-Ray Scattering at the Advanced Light Source

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Small angle X-ray scattering (SAXS) is a technique used by structural biologists to observe the conformations, assembly and shape changes associated with the function of macromolecules in solution. The brevity of sample preparation, exposure time, data acquisition and solution structure modeling furthers SAXS as a high throughput technique. These advantageous qualities can be seen through the analysis of two sample proteins. The design of a multi-well sample cell increases the number of experiments that can be performed, while reducing the accumulation of residue from continued use. Sample cells of varying thicknesses are interchangeable to optimize the scattering intensity based on absorption properties. Not only does the quality of data collection drastically improve, but from a biological standpoint it enables a reduction in the concentration of protein needed for an experiment.

Development of a Simulation Program for Photovoltaic and Wind Integrated CAES Facilities

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Increased interests in the use of renewable energy sources, including Photo Voltaic (PV) arrays and wind turbines, have brought much attention to their effective deployment. With both wind and PV energy sources, intermittency and output variability serve to complicate their successful use in a plant setting. Integration with a Compressed Air Energy Storage (CAES) facility may provide a means to overcome this hurdle by storing excess energy as compressed air for generation during times of greater power demand; however, this integration has yet to be effectively modeled. In this investigation, a CAES plant model was developed through thermodynamic analyses of the turbomachinery from an existing, non-PV/Wind integrated CAES plant in McIntosh, Alabama. The thermodynamic plant model was then coded into a simulation program using Visual Basic for Applications (VBA) complete with an interactive user interface and a Microsoft® Excel data exportation module. Insolation data was then taken from the National Renewable Energy Laboratory (NREL) databases and combined with hourly wind profiles generated using NREL's HOMER software. These PV and wind resource data were subsequently integrated into the simulation program with a time-step of one hour. This VBA simulation program allows the user to specify any configuration for a PV/Wind integrated CAES plant with solar and wind data from any time or location, returning the hourly plant operation profile for any duration of time. This software will provide insight on the feasibility of integrated CAES plants as a way to meet baseload or spinning reserve energy demand profiles. Additionally, this CAES plant simulation program could be further integrated into the NREL's HOMER software to yield a powerful micropower optimization model that would aid in the development of worldwide, PV/Wind integrated CAES power systems.

The Development of the Radionuclide Inventory Workbook for Building 315 Vault 40

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The purpose of this project was to produce an Excel document containing sets of accurate and complete information for the nuclear material inventory of Argonne National Laboratory's Building 315 Vault 40 storage cells. Vault 40 has information compiled into a Microsoft® Excel spreadsheet to use as a baseline reference. Compliance and threshold standards were factored into the data collection. This information has bolstered the Radionuclide Inventory Workbook (RIW) that will track the de-inventory of Vault 40. In addition, each workbook is designed to perform Hazard Category and Pu-239 Fissile Gram Equivalence (FGE) calculations and other desired computations. An outgrowth of the study was the development of an RIW Users' Guide that explains the different types of calculations and markings within the workbook. The guide streamlines the editing of the RIW and adds an extra level of data security. The guide gives instructions for editing data and warnings specific to the different tabs in the workbook. While Microsoft® Excel is a straightforward program to use, care must be taken to ascertain that data are not accidentally lost or altered. The guide makes the user aware of the different types of errors that could potentially result while editing the RIW. The RIW effectively generates and verifies Criticality Control Area postings for the individual storage cells. The RIW underwent a verification and validation process and

has become an essential document for tracking the de-inventory of Vault 40. Presently, only the Vault 40 Facility Manager and Custodian have access to the RIW. While the official inventory database for Vault 40 is the Local Area Network Material Accounting System operated by the Security and Counterintelligence Division Materials Control and Accountability personnel, a separate inventory workbook was needed for Hazard Category and FGE calculations.

Geographic Information Analysis for Wind Resource Assessments and Cost Path Optimization

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Twenty-three states have committed to developing more renewable electric generation technologies in the next 10–15 years. There is a growing need for analysis tools to estimate the cost associated with interconnecting future wind farms to the existing electric grid. In this study, resource assessment tools were implemented that first estimated the available wind resources in terms of installed capacity for the state of Washington. The capacity was a function of area within a proximity to existing bulk power transmission lines. For estimating the cost associated with connecting a future wind energy site, an optimal routing tool was used in a graphical information system (GIS) to determine the least-cost path from a future site to the existing grid. A cost function was defined which based transmission line construction on terrain, slope, distance and land-use. The resulting assessments showed the total potential capacities of wind farms within a range of 5–15 km from existing power lines. The optimal routing function accurately estimated the costs of building transmission lines, and it clearly showed the ability to find the least cost path; the paths created avoided high cost zones such as mountainous terrain. The study was a stepping stone for larger and broader applications such as the development and optimization of other natural resources. Other projects might include cost analysis of building new highways and laying oil pipelines underground. With the majority of wind located in the Midwest, the hope in the future will be to do large scale assessment and analysis on future wind farms within those states.

Monitoring Building Power Usage

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A typical building's energy usage is dominated by the use of electricity and with the growing need to conserve energy, accurate monitoring of power is becoming a necessity. Many buildings on the Argonne National Laboratory site have analog power meters that require personnel to physically read the meters resulting in inefficient use of manpower. One objective of this project is to convert existing analog power meters to ones that are digital and monitored remotely. By converting to a remote monitoring system it will be possible to monitor many buildings from a centralized location and work towards lowering Argonne's power usage. To accomplish this goal the needs and requirements of installing a digital meter that can be read remotely needed to be investigated. The meter must measure voltage, current, the power factor and the power usage and have Ethernet capability so it can be connected to the Metasys system, a system which will serve as the online building management system to consolidate information from various buildings. The meter chosen is from the Schneider Electric ION series because of the information it provides and its compatibility with Metasys. Another part of this project is to evaluate Argonne's power consumption and demonstrate that Argonne National Laboratory can effectively decrease power usage. By performing experiments, such as having employees shut down their computers over the weekend, one can determine how much electricity can be saved with computers shut down. The conclusion of this evaluation is that while power used over night and over the weekends is lower than that used during the day, the reduction of power from computers shutting down is not necessarily the primary factor in the reduction. A more in-depth evaluation is needed. This project will prove beneficial to Argonne by the implementation of new digital power meters and suggested ways to conserve electrical energy.

Reactor Design for Double Diffusion Experimentation

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Strontium-90 (⁹⁰Sr) is a uranium fission product, a by product of nuclear energy production. The radionuclide ⁹⁰Sr is a contaminant of significant concern at Idaho National Laboratory and other Department of Energy (DOE) sites. The radionuclide is chemically similar to calcium, allowing the body to readily uptake it. However, this affinity for calcium also makes it favorable for ⁹⁰Sr to co-precipitate with calcium

carbonate (CaCO_3), a naturally occurring mineral. In addition ^{90}Sr has a relatively short half life of 29.1 years. If ^{90}Sr can be bound up in a stable CaCO_3 precipitate, in a few hundred years the concentrations will be reduced by 99.9% while preventing the contaminant from migrating into groundwater. The success of in situ remediation depends on being able to accurately predict and control the precipitation of ^{90}Sr and CaCO_3 in the subsurface environment. Unfortunately the subsurface is a less than ideal reactor for controlling chemical reactions. It is often heterogeneous, not fully characterized, and limits mixing to diffusion and dispersion along chemical gradients. Due to this poor mixing, volume averaged rates are likely to be inaccurate and inapplicable. The altering of flowpaths as precipitates form further complicates mixing. The goal of this project is to develop a reactor where the precipitation of CaCO_3 can be monitored under conditions simulating the diffusion driven, poorly mixed subsurface environment. Spatial and temporal changes in subsurface conditions due to deposition of mineral phases will be noted. A double diffusion reactor was designed and built by linking two 1L reservoirs with a small diameter glass tube about 5 cm in length. Each reservoir was then filled with either calcium chloride or sodium carbonate solution. To help prevent advection through the column, various gel configurations were tested. The gel was optimized to provide a minimum reduction in the hydraulic conductivity while still preventing advection. Testing showed that the gel was effective at limiting mixing to diffusion only, but all the gel configurations tested slowly began to dissolve and were not stable for more than a day once put into the reactors and immersed in water. Additional sand-filled columns simulating subsurface media were successfully designed, built and operated in the reactor. While time restraints prevented further testing with the reactors, they were successfully built allowing for additional experimentation in the future.

Nitric Oxide Emissions Conversion to Load-Specific and Distance-Specific Units Methods and Impact on Reported Results

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The use of hydrogen as an internal combustion engine fuel is being researched because of its favorable physical properties. Research engineers are seeking to reach certain targets in order to comply with U.S. Department of Energy (DOE) standards. DOE has set challenging goals, aiming for 45% peak brake thermal efficiency and nitric oxide (NO_x) emissions as low as 0.07 g/mile. However, NO_x emissions are measured in parts per million (ppm) at the emissions bench, and the conversion is not easily done or readily available. Therefore, most researchers choose to report NO_x emissions in ppm, which can be misleading and disadvantageous. This paper shows two methods of calculating load-specific NO_x emissions, which can then be converted to distance-specific units. The first method uses the balanced molecular equation of hydrogen combustion, while the second one uses the measured oxygen, hydrogen and nitric oxide content in the exhaust to calculate the volumetric percentages. The two methods both consider humidity and water flow, pertaining to an experimental water injection mechanism. After analyzing numerous parts per million versus grams per mile plots, some trends stand out. There is a high linear correlation between similar tests at the same load point. However, the linear correlation is unique to each engine and load point. Therefore, one cannot compare different engines or different load points when NO_x is reported in ppm, a serious disadvantage. Also, NO_x emissions reported in ppm can be deceiving, showing a low volumetric concentration but, in fact having a high grams per mile reading. Though a conversion to grams per mile is not necessary at all times, it prevents emissions readings from being specific to each engine and load point; and by using simplifying assumptions, it allows research engineers to see how close or far they are from the DOE NO_x target.

Modern High Flux Isotope Reactor Safety System

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Many components of the Reactor Safety System (RSS) at the Oak Ridge National Laboratory (ORNL) High Flux Isotope Reactor (HFIR) are 1960s vintage. Thus they are becoming increasingly more difficult to maintain or replace. The objective of this study was to design, construct and test a new, state-of-the-art, computer-based system to replace the HFIR's current RSS. The concept for a new RSS is the design of a digital Programmable Logic Controller (PLC) equipped with algorithms designed to replicate the calculations and outputs of the original analog equipment. The PLC will use existing monitored plant parameters as inputs. The algorithm uses inputs of data on heat power (in megawatts) and actual measured neutron flux over time to determine a corrected neutron flux level in relation to the more accurate heat power readings. Testing of the new PLC system demonstrated

that, with identical inputs, the algorithm in the PLC reproduced the results of the present system. The PLC has self-diagnostic capabilities, which will make the equipment easier to monitor. Using this state-of-the-art system will facilitate system maintenance, increase system reliability and reduce the time and costs to maintain and troubleshoot HFIR operations.

An Electricity Market Complex Adaptive System (EMCAS) for Energy Planning

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Energy planning is one of the most critical issues today. Consequently, it is imperative to use decision analysis tools to help project and determine future energy needs, particularly for electricity generating systems. The Wien Automatic System Planning (WASP) program, developed by the International Atomic Energy Agency (IAEA) is an example of system planning software in use today. The tool allows for decision makers to study the development of an electric generation system and to determine appropriate technology for long term expansion. WASP has been used globally for the past 30 years. Unfortunately, recent changes in the power industry, notably privatization and restructuring, have altered the way investment decisions in new power plants are made. Therefore, a new tool termed an Electricity Market Complex Adaptive System (EMCAS) has been developed at Argonne National Laboratory to study power system expansion in traditional as well as restructured power markets. EMCAS is useful in planning short-term operations and long-term system expansions. The software uses a probabilistic dispatch algorithm to calculate prices and profits for new candidate units in different future states of the system. The objective of this project is to analyze EMCAS. The goal is to produce results under a variety of scenarios and compare them with results from the WASP model in order to gain a deeper understanding of energy generation systems and how they are impacted by future investment decisions. This is particularly valuable for studying a system's long-term expansion. This study analyzes a simple case scenario using both EMCAS and WASP programs. The EMCAS model simulates investment decisions of decentralized generating companies. When fuel prices are raised, it affects the decision-modeling results of EMCAS. Moreover, when competition is added it improves the representation of actual markets in EMCAS. An analysis of the results show that new insights can be gained by using EMCAS. Future work will focus on examining additional drivers that affect multi-agent investment decisions using the EMCAS software.

Baseline Performance Modeling and Hydrofoil Survey for an Axial-Flow Tidal Turbine

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The National Wind Technology Center (NWTC), a division of the National Renewable Energy Laboratory, has expanded its research into ocean renewable energy technologies. The NWTC's current interest is in the preliminary design and baseline performance modeling of axial-flow tidal turbines. These axial-flow tidal turbines operate on many of the same principles that wind turbines do and are in a class of "zero-head" hydropower which uses the kinetic energy of flowing water to drive a turbine. This paper focuses on use of the NWTC's existing wind turbine performance code (WT_Perf), which relies on Blade Element Momentum theory, to analyze an existing tidal turbine rotor. The assumption was made that as long as a cavitation is introduced as a constraint on a wind turbine type model, the Blade Element Momentum theory is still valid and reasonably realistic results would be achieved. Once the modeling input parameters were verified to accurately represent the tidal turbine configuration, the code's accuracy was verified by comparing the code's predictions to experimental test data. Variations of rotor geometry and hydrofoil options were then modeled in order to find configurations for optimal performance. Candidate rotor configurations and hydrofoils were judged on their favorable characteristics for energy capture at low flow speeds, hydrodynamic stall regulation and for resistance to cavitation. The relative performance of the candidate hydrofoils were then compared to the performance of the baseline turbine configuration. Agreement between the measured and predicted values were excellent for flow speed less than the rated speed of the turbine. As the flow speed approached and exceeded the rated speed of the turbine, there began to be deviation between the measured and predicted values. Possible reasons for this deviation may be cavitation, dynamic effects, modeling of the turbine wake and also experimental error in the measured values. Recommendations for improvement to the WT_Perf hydrodynamic model and cavitation prediction models were also discussed.

Life Cycle Cost Analysis of Battery Storage for Regulation Services

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To manage fluctuations in the electric supply caused by adding more intermittent renewable energy resources, regulation services will require more capacity. Commonly, combustion turbines (CT) are used to provide regulation services in the electric grid. Batteries are an alternative technology for regulation services. Using electric vehicles for regulation services has received public attention. This concept, usually referred to as Vehicle-to-Grid, is based on the assumption that the battery in the vehicle could be utilized for regulation services while the vehicle is parked for long periods during the day. This research analyzes the cost competitiveness of replacing the CT technology with stationary batteries. The comparison was based on a 20-year life cycle cost (LCC) and used the cost, performance and life degradation characteristics of currently available batteries designed for transportation purposes. The results of the LCC analysis suggest that current battery technology would reduce emissions but would be more expensive than CTs. However, if battery technology achieves the cost and performance target set by the U.S. Advanced Battery Consortium for 2016, then replacing the CTs with battery storage would provide significant savings.

* Technical Documentation of TTB and LTB Beam Stops

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The beam stops in the Tandem Van de Graaff to Booster (TTB) and Linear Accelerator to Booster (LTB) beam lines are part of many subsystems in the Collider-Accelerator (C-A) complex at Brookhaven National Laboratory (BNL). Beam stops are used as an initial safety response in case beam-control parameters stray from the required specifications. They perform this task by blocking the path of the accelerator beam during accelerator operations. Documentation of these subsystems is desired in the C-A complex at BNL to centralize and consolidate information making it readily available for C-A department staff, particularly newly hired employees. I gathered information on the location, construction and operation of the beam stops from C-A staff members, manufacturer's manuals and electrical schematics. With this information, I authored a document detailing four important aspects of the LTB and TTB beam stops: their locations, the physical aspects needed to recognize the beam stops themselves, how they function, mechanically and electrically, and the necessary requirements for entry. This work is a small component of a larger effort to document the various systems and subsystems in the C-A complex in order to provide information to employees, who often work in hazardous areas, so that they can work as safely and quickly as possible.

An Analysis of the Fiducial Timing System for the Linear Coherent Light Source Radio Frequency Timing System

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In preparation for the completion of the Linear Coherent Light Source (LCLS) in 2009, many upgrades are being considered for the Stanford Linear Accelerator (linac). The radio frequency (RF) timing system is of particular importance to LCLS, because it is the standard reference for the linac's electron beam, and is used to trigger automated events along the two mile linac. Two primary questions under consideration are the feasibility of using a missing pulse triggering scheme and the potential benefits of upgrading to a bipolar fiducial pulse. To evaluate potential changes to the RF timing system, a simulation of the Main Drive Line (MDL) system response and fiducial pulse was developed. Using the MDL model to simulate the effect of the MDL on the monopolar fiducial pulse and the bipolar fiducial, it has been confirmed that upgrading to the bipolar pulse would provide no significant benefit to the RF timing system. For the purpose of timing, the monopolar pulse and the bipolar pulse are interchangeable. The key difference between the pulses can be observed in sector 0 and sector 30. The key difference is that in sector 0 the bipolar pulse has 2.0079 times the power of the monopolar pulse; and in sector 30 the power ratio is approximately 0.4972.

The sector 30 power ratio is a compelling argument in favor of the monopolar pulse. Because the majority of the power for the monopolar pulse comes from low frequency components in the Fourier transform of the signal, the nonlinear response of the MDL causes the wave form to spread and encroach on the cycles of the carrier signal following the pulse. However, this is not a major issue for the purpose of detecting a trigger. Because of the power of modern signal processing techniques, a monopolar pulse is effectively equivalent to a bipolar pulse for the purpose of timing, meaning the negative aspects of both signals can

be handled with equivalent amount of effort. Using the MDL model, it has also been confirmed that a missing pulse is precluded as a possible triggering scheme for the monopolar fiducial pulse due to pulse spreading. The bipolar fiducial pulse cannot be used in a missing pulse configuration due to severe attenuation. Future work in the analysis of the RF timing system would include adding frequency dispersion to the MDL model, building a prototype bipolar pulser, and refining the MDL model.

Wireless Traffic Density Counter

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The objective of this project is to develop a wireless traffic density counter to aid in pre-disaster emergency evacuation. The counter will be small, lightweight, easy to deploy with minimal set-up or calibration, and relatively inexpensive and easy to maintain, requiring very little attention over extended periods of time. If an event occurs similar to Hurricane Katrina, such a device would provide a means of monitoring not only the main evacuation routes but also secondary routes to aid in expeditious and effective evacuation. The following factors were considered: type of sensors, type of wireless transmitting device, what information would be most useful, and deployment methods. The sensor choices considered were: Hall Effect, magnetic proximity, ultrasonic and passive infrared (PIR). The wireless devices considered were: Archrock Wireless Sensor Nodes, Rabbit Technologies Zigbee Application Kit and the Texas Instruments MSP 430 eZ430-RF2500 Development Tool. The most useful information was determined to be number of vehicles, speed, size and type. The methods of deployment that were considered included: gluing the unit to the road, embedding it in the road, mounting it under a bridge and mounting it on a sign beside the road. Emphasizing low-power consumption, PIRs connected to TI MSP430's mounted on a sign beside the road to measure speed and count the number of vehicles was selected. The next step was to build a test circuit based on logic gates. The circuit has no memory and its only output is 16 LEDs. The circuit uses one PIR to start a counter and one PIR to stop the counter. After the counter is stopped, the LEDs will either be on or off, indicating a binary number combination that can then be translated into a decimal number and converted to miles per hour. The reaction of the PIRs and count were consistent based on laboratory conditions. The next phase of the project will be to connect and program the automated circuit and perform final testing. In terms of pre-disaster emergency evacuation, a system like this will be invaluable in aiding the safe and expeditious flow of thousands of people. It will have an impact on more than just hurricane evacuation. Other applications could include use at the perimeter of large urban areas in the event a disaster requiring evacuation, such as chemical spills, nuclear hazards, wildfire, etc. occurs.

The Use of Polypropylene Heat Exchangers in Oil-Burning Boilers

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Condensing boilers achieve high thermal efficiency by recapturing latent heat in the flue gases. The condensate that forms is corrosive, requiring stainless steels. Plastics, an alternative, meet the temperature requirements, but have low thermal conductivity. In this project, potential use of nanoparticles to improve the thermal conductivity of plastics and the heat transfer conditions in heat exchangers were studied. Metal tubes used in oil boiler heat exchangers are not cost effective, not easy to fabricate, corrode and foul. These factors lead to heat loss from flue gases which could be retained to preheat boiler water and improve heating unit efficiency. Polypropylene (PP) is relatively cheap and easy to manufacture, with no corrosion/fouling difficulties. A literature review, calculations and experiments were done to determine if the low thermal conductivity of PP is a major inhibitor when used as a heat exchanger, and if it could be offset through the use of nanoparticles. The thermal conductivity (K) of PP is approximately 0.22 (W/mK), which is low when compared to the metals used in heat exchangers such as Al (K=250 W/mK). Use of nanoparticles such as Talc (30 vol %) can raise the thermal conductivity to 2.5 (W/mK). This is still too low compared to Al. It was discovered that the main inhibitor to heat conduction through the exchanger is not the thermal coefficient, but the thermal convective film between flue gases and the inner wall of the plastic tube. This contributes over 99% of the resistance experienced by the heat exchanger. It was found that nanoparticles had an effect on the exchanger's ability to move heat from flue gases to the boiler water. PP can also withstand the high temperatures of flue-gases since it would contact the cooler boiler water (80 °F) while PP's melting point is 320 °F. The thermal conductivity of PP is not an obstacle. This plastic can withstand the high temperatures it is exposed to. The

use of nanoparticles does not make a significant difference in the ability of PP to recapture waste heat. Thus, it was found that a plastic heat exchanger in an oil boiler is feasible since it is not vulnerable to corrosive flue-gases, as metals are. Plastic heat exchangers can replace metal heat exchangers, resulting in equal efficiency of heat recapture without corrosion effects. Also, experimental work confirmed our previous calculations.

Educational Materials Developed about Biodiesel as an Alternative Fuel at Sagamore Hill National Historic Site

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Biodiesel is a renewable, environmentally friendly "green fuel" that can replace No. 2 fuel/heating oil in traditional space-heating applications. Thus biodiesel, which can be domestically produced from various feedstocks including virgin vegetable oils, waste vegetable oils and animal fats, directly promotes the conservation of our nation's natural resources. There are, however, several combustion and material compatibility characteristics of biodiesel that differ slightly from its petroleum-based counterpart, No. 2 fuel oil. In order to determine the feasibility of using biodiesel in traditional oil-fired space heating equipment, Brookhaven National Laboratory, in conjunction with the National Park Service, began running a blend of 20% biodiesel and 80% No. 2 oil (B20) at the Sagamore Hill National Historic Site in Oyster Bay, NY. The overall purpose of this study was to characterize the feasibility of converting home heating systems to run on biodiesel and to provide the public with educational materials about the benefits of "green fuels" and the use of biodiesel at Sagamore Hill. This summer, the main focus of this multi-year project was to develop these educational materials. First, a tri-fold brochure was developed on Microsoft Word that gave a brief history of Theodore Roosevelt's conservationist efforts, an overview of biodiesel and its environmental benefits, the purpose for burning biodiesel at Sagamore Hill, as well as other important information regarding alternative fuels. After approval from the Public Relations Department of Brookhaven National Laboratory, the New York State Energy Research and Development Agency and the National Park Service, this brochure will be available to the public at the Visitor's Center at Sagamore Hill. Additionally, a PowerPoint presentation on the use of biodiesel at Sagamore Hill was created to provide educators with a more in-depth look at biodiesel and its properties as well as President Theodore Roosevelt's contributions towards conservation in the United States. In order to make this presentation as versatile as possible for educators, extensive use of both history and science concepts was utilized. The goal is to have this PowerPoint presentation available on the Internet at the Sagamore Hill National Historic Site website as soon as possible so that teachers from all over the nation will be able to access the information.

Engine Test Cell Preparation and Experimental Apparatus Design

Ryan Thorpe (UNIVERSITY OF COLORADO—BOULDER, BOULDER, CO 80310), Steve Ciatti (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). Biodiesel has been receiving a lot of attention lately with regard to its use as a transportation fuel. Scientists at Argonne's Center of Transportation Research will begin experimenting with biodiesel/butanol fuel. To do research on the biodiesel/butanol fuel a General Motors (GM) 1.9 L diesel engine test cell must be fully operational, safe and easy to use. Making the engine fully operational will require engine disassembly and diagnostic tests. The engine was disassembled to set proper timing and diagnostic tests were performed to identify Diagnostic Trouble Codes (DTCs). Unfortunately, the GM 1.9 L engine still failed to fully operate. Since the Engine Control Unit's (ECU's) programming is GM's proprietary information, its architecture is locked making it difficult to troubleshoot engine problems. To fix that problem an open architecture ECU will be purchased, allowing researchers to fully monitor ECU activity. That could result in the GM 1.9 L engine test cell being fully operational in the future. While preparing the test cell, an optical pressure vessel was designed to explore a novel optical diagnostic technique. If this technique becomes well understood temperature, pressure and molecular species can be discerned in temporal resolution from an engine operating at full load. To safely design the pressure vessel, many pressure vessel code handbooks had to be used. These handbooks contained material strength data and solid mechanics formulas that were essential to the design process. The material data and solid mechanics formulas enabled the designer to specify the thickness of an optical quartz window to prevent sudden fracture. The resulting quartz window thickness was calculated to be 7.7 mm. Although 7.7 mm is thicker than most optical quartz windows it is feasible because nearly 25 bar of pressure, an unusually high pressure, will be acting on it. The final pressure vessel design was

simple, compatible with common laboratory fittings and provided a factor of safety of 10 to resist a pressurized explosion. Future work could consist of applying this technique to a production internal combustion engine. That would allow the combustion process to be studied under realistic operating conditions.

Arc Flash Analysis for Laboratory-wide Equipment Rating

Jonathan Todzia (RENSSELAER POLYTECHNIC INSTITUTE, TROY, NY 12180), Swapna Mukherji (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). At Brookhaven National Laboratories, all electrical equipment is subjected to rating for arc flash hazards in order to conform to National Fire Protection Agency (NFPA) 70E-2004 standards. The purpose of the analysis and eventual labeling, part of an ongoing project, is to safeguard all workers against both electric shock and arc flash dangers by making them aware of the risk at hand. Labels will be affixed to all equipment warning all workers of the hazards involved. To begin the analysis, data was obtained from equipment on site via manufacturers' labels, existing drawings, electricians, etc., to create one line drawings of each building or group of buildings. Information such as panel ampacity, fuse and breaker ratings, feeder lengths and sizes and transformer ratings were all needed to produce accurate one line diagrams. The incident energy, required personal protective equipment (PPE) and safe boundary conditions were calculated from the information in these drawings. The drawings and calculations were performed utilizing SKM PowerTools software which also provided the final rating of each piece of equipment. The ratings consist of a number from 0 to 4 (4 being the highest danger) which corresponds to the level of PPE required to operate the equipment safely. The entire site's electrical power system needs to be examined. With roughly fifty buildings completed this summer the project is about 80% complete. Upon the completion of the project, all equipment on site will be given new labels stating any arc flash hazards in addition to the proper PPE required for safe operation.

*** Simulating a Radio Frequency Cavity in Real Time Using a Field Programmable Gate Array**

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Fermi National Accelerator Laboratory uses radio frequency (RF) cavities to accelerate particle beams to high energies. These cavities are controlled using complex electronic equipment. Field programmable gate array (FPGA) based real-time simulators are useful for developing and testing such equipment. To model the response of an RF cavity in real-time, a discrete difference equation in the firmware of a Xilinx® XtremeDSP Development Kit (Virtex-4 Edition) was implemented using VHDL Hardware Description Language (VHDL). A user interface was created in MATLAB using C language MEX-files to communicate with the firmware. After the FPGA was configured, the real-time output was compared to offline calculations to verify that the difference equation was implemented correctly. The output was as expected with the exception of some minor problems. The core was successfully completed, but some additional firmware components would be required for a fully functional simulator.

Thermal Analysis Validation through Thermal Imaging

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All beam-interacting components in the Advanced Photon Source (APS) require thermal and stress analyses, using computer aided software, prior to fabrication and installation to ensure that thermo-mechanical limits are not exceeded during operation. Common questions asked are how accurate these results are and if adequate operational safety margins have been incorporated in the component design. This study was conducted to validate that the theoretical findings resulting from computer thermal simulations match the experimental findings for a GlidCop® (alumina oxide dispersion strengthened copper) block sample as it is heated by the APS X-ray source. The block is water cooled and uses wire coil inserts for enhanced heat transfer. The U-shaped water channel in the block uses forced convection to keep the block from overheating. The heat transfer coefficients for this configuration are experimentally determined as a function of coolant flow rate. The emissivity of the test piece is experimentally determined as a function of temperature, surface finish and orientation. These parameters are fed into the computer simulation model and compared to experimental results obtained at the beamline. An infrared camera is used to measure the surface temperature of the block and the enthalpy rise of the water is measured to determine the total power absorbed in the block. When compared, the final results confirm that thermal simulations provide fairly accurate results and can be used with confidence in the design of new beamline components.

Analysis of the ITER Draining and Drying System

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The purpose of the International Thermonuclear Experimental Reactor (ITER) project is to build a fusion reactor that will serve as the basis for designing future power plants to produce electricity. Fusion energy would reduce the emissions of greenhouse gases into the atmosphere, which should slow global climate change. The ITER project involves collaborators from many countries; the various countries have different project responsibilities. One of the tasks assigned to the United States is that of managing the water cooling system. This summer's research involved verifying engineering designs for the draining and drying systems that must be done for the effective procurement of the process experiment for this project. Modeling and simulation programs in FLOW (an ORNL software platform) were used to accomplish this. I prepared a module in FLOW that simulates compressors. The module consisted of code, written in Python, that uses the temperature, pressure and mass flow of the incoming stream, as well as the adiabatic efficiency and outlet pressure. The module uses these data as inputs, and calculates the volumetric flow rate, the adiabatic head size, density and power. Results from the FLOW simulations corroborated several of the design parameters. In fact my modeling analysis almost exactly corroborated modeling analysis performed earlier by the project team. As a teacher, my students will be asked to build a flow sheet showing the way energy flows through an organism, similar to the way flow sheets are made to show the flow of energy through the ITER project.

Tribological Evaluation of Multicomponent Nanoparticle-based Lubricant Additives

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Friction and wear are significant sources of energy and material losses in mechanical processes, and thus lubrication, which can mitigate these losses, is a principal focus of efforts to improve energy efficiency and mechanical durability. Multicomponent nanoparticle-based additives have shown promise as an environmentally neutral alternative to the damaging chemical additives that are currently used to enhance lubrication by reducing friction and wear. This investigation focused on inorganic-organic nanocomposite concentrate lubricants consisting of MoS₂-based inorganic nano-solid lubricants that are intercalated and encapsulated with an organic Canola oil medium. These lubricants were provided by NanoMech, LLC and were evaluated under a Department of Energy (DOE) funded project with Caterpillar and the University of Arkansas. A trial on a pin-disk tribometer setup with a five-newton load over a range of revolutions per minute (1–50 rpm) was used in order to evaluate the performance of each lubricant in the hydrodynamic, mixed and boundary regimes of lubrication. The performance of the lubricants under prolonged extreme conditions was assessed by using day-long, low-speed (1 and 3 rpm) testing. After each test, an optical profilometer was used to analyze wear. In the variable-speed test, compared to the base oil alone, the additives lowered the coefficient of friction by over 50% for speeds over 10 rpm and by approximately 10–30% for lower speeds. Moreover, with the additives, the contact surfaces showed considerably less wear. For both long-term tests, both additives had lower maximum coefficients of friction than that of the base oil, but their steady-state coefficients were approximately 10% higher for the 3-rpm test and 10–30% higher for the 1-rpm test. Furthermore, the additives either did not affect or increased the amount of wear. While the nanoparticle-based additives reduce friction over the short term, the results suggest that over time they cause wear that increases friction. As this investigation continues, more trials will be performed to confirm these initial results, to explore the differences between the additives, and to examine their performance under various conditions. The preliminary results show potential, so the lubricants will be tested in a block-on-ring tribometer, which more closely simulates engine conditions, and the mechanisms by which these environmentally innocuous additives reduce friction and wear will be analyzed.

Phase Inversion Behavior of Liquid-Liquid Dispersion in Centrifugal Contactors

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Phase inversion is a phenomenon in which the dispersed phase in a liquid-liquid dispersion, such as oil-water dispersion, becomes continuous, and the continuous phase becomes dispersed. It occurs in liquid-liquid extraction systems in various applications

including hydrometallurgy, alternative fuel reprocessing and chemical separations. The goal of this project is to better understand and improve the performance of centrifugal contactors. Phase inversion is determined by the physical properties of the liquids, geometrical factors and operating parameters. In experiments reported here, two immiscible fluids of different densities (an aqueous solution and an organic solvent) were fed into a centrifugal contactor from different inlets. The two fluids form a dispersion by means of shear rate generated in the contactor before being separated by centrifugal force. The fluids then exit through the designated outlets. In this project we focused on the ambivalence region where the role of each phase is interchangeable. If the volume fraction of the organic phase is greater than the upper bound of the ambivalence region, then the organic phase is always continuous and the aqueous is always dispersed. This means that the dispersion consists of water droplets in oil. Conversely, if the volume fraction of the organic phase is less than the lower bound of the ambivalence region, the aqueous phase is always continuous and the organic is always dispersed. A conductivity probe placed inside the rotor inlet of the centrifugal contactor is used to determine phase inversion. The operating parameters that we manipulated included rotational speed of the rotor of the contactor and flow rates of the two phases. In this experiment, five agitation rates were used; these ranged from 3000 to 4200 rpm. For the lower boundary curve we started the flow rate at 200:200 organic to aqueous, which falls within the ambivalence region. The organic flow rate then was reduced and the aqueous flow rate was increased stepwise until phase inversion occurred. For the upper boundary curve, we started the flow rate at 100:300 organic to aqueous. The organic flow rate was increased and the aqueous flow rate was reduced stepwise until phase inversion occurred. Each point was tested three times to characterize reproducibility. Results showed that agitation speed does not affect the phase inversion point for the conditions used: the phase inversion point remained similar throughout the experiment.

Rheological Studies on Physical Simulants of Hanford Legacy Tank Waste Using the Anton Paar HVA 6 Automated High Shear Capillary Viscometer

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The 53 million gallons of nuclear and chemical legacy waste stored in the 177 underground tanks at the Hanford Site, a former plutonium production complex in southeastern Washington State, is one of the foremost environmental concerns affecting the world today. To remediate the site, the Department of Energy, Bechtel National Inc. and the Pacific Northwest National Laboratory are designing, commissioning and constructing the Waste Treatment Plant (WTP) to vitrify the waste and allow for safer storage. A principal concern of the project is how to transport the waste from the tanks to the WTP. To this end, engineers have analyzed and characterized the tank waste rheology for each individual tank. To efficiently and effectively test rheology data, physical simulants of actual waste were synthesized and analyzed. The Anton Paar HVA 6 Automated High Shear Capillary Viscometer was used to determine the material's law of the sample from measured parameters. Through calculation, the relationship between viscosity and shear rate could be obtained. Also used in the rheology analysis were the Anton Paar MCR 501 Rheometer with pressure cell unit and the TA AR-2000 Rheometer with a pressure cell unit. Hanford Site tank wastes have exhibited both Newtonian and non-Newtonian fluid properties. To account for these different properties, distilled water and viscosity standards from the Brookfield Engineering Laboratories, Inc., of 0.1 centipoises (cP), 48 cP and 98.2 cP were tested. For a much thicker standard, kaolin clay mixtures of 5%, 10% and 15% solid by weight were also tested. With the data, subsequent viscosity curves were created digitally. Initial reports indicated that the Anton Paar HVA 6 Automated High Shear Capillary Viscometer may not be prepared yet to give results that will yield influential data. Viscosity reported for water at room temperature was an average of 0.50 cP and varied wildly. This reported value was below the known value of 0.89 cP for water at room temperature, confirmed by the two other rheometers. The machine is sensitive to air bubbles, and the presence of air bubbles was noticed in the capillary during testing despite efforts taken to remedy this situation. This would have confounded the results of the experiment. Future calibration and machine optimization is recommended for the Anton Paar HVA 6 Automated High Shear Capillary Viscometer. If fully operational, this machine would be a vital asset and provide the ability to calculate rheology data and higher shear rates.

Environmental Science

*** Microbial Community Mapping of Long Island's Pine Barren Forest Soil**

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Management of any ecosystem requires information on the flora and fauna present in the environment. Current management plans for terrestrial ecosystems are based mainly on macrofauna. Even though microorganisms are critical for maintaining the balance in an ecosystem, no information is available on the types and behavior of microorganisms in the soil of the Long Island Pine Barren Forest. Thus, the existing management plan for this ecosystem does not consider the influence of the actions on the microbial diversity. In the first study of its kind, we mapped the Long Island Pine Barren Forest (LIPBF) soils based on their microbial, community-level, physiological profile (CLPP). Soil samples were collected from different parts of the forest and upon preparation of the inoculum, BIOLOG EcoPlates were inoculated. A clustering analysis based on color intensities illustrated that the entire LIPBF can be divided into four different clusters at every horizon. However, the physiological response of the microbial community at each horizon and cluster was different. No correlation between sampling sites and the physiological profile was obtained based on vegetation or geographical location. In conclusion, comparing the physiological profile of the microbial community from each horizon, one can make a list of substrates that are utilized more throughout the LIPBF. Further studies need to be carried out to test this hypothesis in the future.

*** Characterization of Attendant Shelf Clouds over the Tropical Western Pacific Warm Pool**

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Research in the field of atmospheric science improves not only our understanding of atmospheric interactions, but also our abilities to predict meteorological and climatic events. Using data from the Department of Energy's Atmospheric Radiation Measurement (ARM) program, the following research characterizes one aspect of our atmosphere: attendant shelf clouds (ASC). Measurements taken over the tropical western Pacific (TWP) warm pool (WP) region (off the north-eastern Australian coast), often show the presence of thin clouds at and around the freezing level stable layer. Typically, these shelf-like clouds extend from cumulo-nimbus or cumulo-congestus cells. Our characterization of this cloud type began by sampling information from an array of data products developed through the ARM program. The data were then organized using a collection of original computer scripts. Through analysis of the resultant material, ASCs were determined to occur approximately 15 percent of the time, to come about in the presence of slightly more than average stable layer above the freezing level, to contain an average of 0.00521 cm of liquid water, and to induce a cloud forcing of -237.22 W/m^2 . After examining our results, we found that attendant shelf clouds occur frequently enough to be considered a normal aspect of tropical meteorology. Identification of these parameters of ASCs allows us to incorporate them into a more complete understanding of our atmosphere. Further, with this increased knowledge, we can better critique the verisimilitude of computational models of our atmosphere and, hence, improve our predictive abilities.

Examining the LC50 of *Hyalella azteca* When Exposed to Varied Concentrations of Silver Nanoparticles in a Static Freshwater System

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The use of silver in consumer products is receiving renewed interest due to the increased effectiveness of silver as an anti-microbial agent when in nanoparticle form. Silver nanoparticles are an additive today in common items such as bandages, socks, underwear, and even items like electric razors and computer keyboards. With this renewed interest comes concern about the effects of silver nanoparticles on the environment. This study examined the effects of exposing the benthic, freshwater, amphipod *Hyalella azteca* to concentrations of silver nanoparticles during a 96 hour static test. The physical setup for the experiment consisted of 125 mL containers with 7.5 g of Accusand 20/30, 75 mL of groundwater/silver nanoparticle solution, and five amphipods. The silver nanoparticles ranged in size from 30–200 μm and the concentrations of silver nanoparticles tested (measured as total Ag) were unamended groundwater, 0.4, 4, 41 and 296 $\mu\text{g Ag L}^{-1}$. The activity of the amphipods was noted every 24 hrs, and percent mortality was determined at the conclusion of the study. The only concentration

where mortality was observed was in the highest concentration, 296 $\mu\text{g Ag L}^{-1}$, where 20 of 25 amphipods were observed dead at 48 hours, and no additional mortality was recorded by 96 hrs. The lethal concentration killing 50% (LC50) of the amphipods was calculated to be 141 $\mu\text{g Ag L}^{-1}$ using a graphical method. The results of this study showed that amphipods were tolerant to a higher concentration of silver nanoparticles than that reported in the literature for ionic silver exposures. The analysis of the silver nanoparticles in groundwater indicated that most of the silver was aggregated (between 14 and 45% of the silver was able to pass through a 0.45 μm filter) and not present in ionic form. The results of this study indicate that silver nanoparticles in the freshwater environment may not be as toxic as ionic silver to benthic aquatic organisms.

The Effects of Physical and Chemical Water Quality Parameters on the Distribution of Aquatic Invertebrates within the Carmans River on Long Island, New York

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While the Carmans River is one of a few pristine aquatic ecosystems on Long Island, roadside runoff, fertilizers, septic systems and groundwater contaminants all threaten to degrade its condition. All of these factors directly affect water quality and the distribution of aquatic invertebrates, which, in turn, affect higher trophic levels. Sensitive populations such as invertebrate species serve as indicators of biological integrity and can be useful for identifying problems in water quality. This research is the initial investigation of a longitudinal study and will be used for planning mitigation projects. The physical and chemical variations in water quality were compared for six different locations and among three habitat types selected along the Carmans River. Water samples taken at each location were then tested in areas of varying water velocities. A Yellow Spring Instruments, Inc. (YSI) 650 MDS water quality meter was used to measure the real-time data for temperature, pH, dissolved oxygen, conductivity, and turbidity. Water samples were analyzed using a HACH Company Digital Titrator and colorimeter. Using a Surber sampler, aquatic invertebrate samples were collected, preserved, sorted and then identified using a compound light microscope and taxonomic keys. Rapid bioassessment, another technique used to assess invertebrate diversity, provided supplementary data needed to create a more accurate biodiversity index. By comparing the data collected from each site, invertebrate distributions were correlated with environmental parameters. The Carmans River and the biodiversity that it supports has been identified as a key natural resource on Long Island by several groups including the U.S. Fish & Wildlife Service, the Environmental Defense Fund, the Nature Conservancy, and the New York State Department of Environmental Conservation. The results from this experiment showed that with movement downstream, the diversity of invertebrates increases with increasing habitat complexity, as expected. Also, from our data it can be concluded that upstream locations are more affected by runoff and other sources of contaminants than downstream locations. Using data from this initial investigation, areas of concern can be targeted for future projects to improve the water condition of the Carmans River.

Comparing Surface Energy Balances for Atmospheric Radiation Measurement Sites

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Solar energy is received and used in various amounts in different regions of the world. The goal of this experiment was to determine how the surface energy balance varied in three regions and how it related to the climate in those regions. Data collected at the Southern Great Plains, Oklahoma site (SGP), the Black Forest region in Germany (FKB), and the Niamey, Niger site (NIM) by the Atmospheric Radiation Measurement (ARM) program were chosen for their variability in climatic patterns. The variability between the sites is primarily a result of latitude, cloud cover, and vegetation on the surface. One of the reasons why climate models are not accurate is because they do not take into account how the various physical geographies influence surface energy balances and thus regional climates. Measurements of the components of the surface energy balance, latent and sensible heat flux and net radiation, were compared between the three sites during the months of June of 2007 (SGP and FKB) and 2006 (NIM). Ground heat flux, generally the smallest term in the budget, was not available at all sites and so was excluded from this study. Closure, or the residual of the measured surface energy balance, was used to determine the accuracy of the measurements. Latent heat flux was

greatest at the FKB site. Sensible heat flux was greatest at the NIM site. Net radiation was greatest at the SGP site. The FKB site had the most latent heat flux because it had dense vegetation that contributed to the formation of clouds and precipitation. The NIM site had the most sensible heat flux because it had less vegetation and more exposed soil, which contributed to a warmer and dryer climate. The SGP site had the most net radiation due to the longer days and the position of the sun associated with the summer season. The results of this study help quantify how the components of the surface energy balance vary with climatic regions, from a warmer, dryer climate like the NIM site to a cooler climate with more precipitation like the FKB site.

Using RNA Interference to Study the Effect of Silencing Aux/IAA Genes on *Populus* Root Growth

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The objective of this study was to identify the effect of silencing genes belonging to the Auxin/Indole-3-Acetic Acid (Aux/IAA) gene family on *Populus* root growth through RNA interference (RNAi). The Aux/IAA family consists of genes which are either suppressed or expressed as early as two to three minutes after auxin application and are referred to as early auxin response genes, regulating several plant growth and developmental processes. By down-regulating Aux/IAA in *Populus* transformants, carbon allocation and partitioning to roots may increase carbon sequestration potential. Increasing the amount of carbon belowground could have a global impact by increasing the amount of CO₂ stored in underground biomass. I used quantitative real-time polymerase chain reaction (qRT-PCR) to measure the level of gene expression for Aux/IAA in multiple transformants from six different gene constructs; Aux 3-1, Aux 3-2, Aux 3-4, Aux 7, Aux 16-1, and Aux 17. RNA was extracted and treated with DNase enzyme to get rid of any remaining genomic DNA (gDNA) that might cause contamination prior to complementary DNA (cDNA) synthesis. Using the cDNA, qRT-PCR was performed to measure the degree of fluorescence emitted by the SYBR® Green molecule when it attaches itself to the double stranded DNA during amplification. The level of fluorescence is then correlated into a relative expression for the target genes. The results of the experiment revealed that the relative gene expression of Aux/IAA in all transformant plants is down-regulated from the transformant control. Aux 16-1 primers consistently produced dimers despite changing primers or reducing primer concentration. Additionally, the transformant control expressed up-regulation from the wild-type control in the Aux 3-1, Aux 3-2, and Aux 16-1 gene constructs; however, the opposite is true of Aux 3-4, Aux 7, and Aux 17 gene constructs. This study concludes that RNAi is an effective method for down-regulating AUX/IAA genes in order to investigate root proliferation in *Populus*, and therefore maybe useful in other applications for silencing gene expression. Suggestions for future research include mutant complementation studies, optimizing Aux 16-1 primers, and research for the effect of environmental factors on gene expression between transformant and wild-type controls.

Principle Components Analysis of Aerosol Mass Spectra

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Earth's climate is greatly affected by aerosols, small particles in the atmosphere, around which all cloud drops form. Our aim is to characterize and visualize the composition of aerosol particles to better understand the effect they have on climate and to represent them accurately in climate models. We are working with data obtained using the Aerodyne Aerosol Mass Spectrometer from a flight of a G-1 aircraft over Mexico City on March 19, 2006. The data set contains the concentrations of components of the aerosol particles in terms of mass-to-charge ratios. We analyzed the composition of aerosols from an urban plume of a mega-city, Mexico City, using Principle Components Analysis (PCA) on the covariance matrix of the data set, and used Singular Value Decomposition to obtain the principle vectors. We also analyzed projections upon the principle vectors of typical factors, like sulfate, nitrate, and hydrocarbon-like organic aerosols, oxygenated organic aerosols, and biomass burning organic aerosols, which are characterized by their spectra. We used Igor Pro software for computation and visualization of the data set. This analysis helped us to understand how the composition of the aerosol particles changes over time and distance from the city. Nitrates, which are produced from car exhaust, are representative of young aerosols. As the air mass moves away from the city and the aerosols age, the concentration of nitrates decreases, and the concentration of organics increases. The dimensionality of the aerosol, how many variables are

needed to describe the aerosol in a statistical simulation for future use in climate models, was investigated. We found that the data set can be compressed into six principle components with 99% of the variance explained, and that it can be compressed very well using just three principal components, explaining 96% of the variance. We conclude that PCA is a powerful tool for analysis, compression, and visualization of an aerosol mass spectra data set. The method has been used here to determine how the composition of the aerosol changes with age during a field experiment. The compression studies suggest that statistical approaches based on PCA have the potential for greatly improving the efficiency of aerosol representation and tracking in climate models.

Distribution of the Iridovirus in Eastern Box Turtles at Brookhaven National Lab

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The Iridovirus is a family of pathogenic disease that affects reptiles, fish, and amphibians worldwide. Currently, there are four documented genera: The Chloriridovirus and Iridovirus (which infect invertebrates) and the Lymphocystivirus and Ranavirus (which infect cold-blooded vertebrates). A recent outbreak of this Ranavirus had been detected on Brookhaven National Lab (BNL) property among the Eastern Box Turtle population. The symptoms of the Ranavirus in Eastern Box Turtles include conjunctivitis, lethargy, oral and nasal discharge, and death. Since New York state considers this species a special concern, a survey was needed to track and record the size and effect of this outbreak. A group of oral and cloacal samples of Eastern Box Turtles was collected on site for DNA. These DNA samples were removed from the swabs using the DNeasy tissue kit procedure. The samples were run through Polymerase Chain Reaction twice to enhance the DNA quantity, and then placed into an electrophoresis gel. Using Geographic Information Systems (GISs), the location of all turtles found was plotted so the distribution of the virus could be seen across BNL. The results came back inconclusive for this experiment. The majority of the testing came back negative, however there was reasonable doubt as to whether the outcome was reliable. Also, there was not enough consistency in the GIS plotting to be reasonably sure of the Ranavirus' movements.

* A Distribution Survey of the New York State Threatened Banded Sunfish (*Enneacanthus obesus*) Conducted in the Peconic River Drainage on Long Island, New York

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The New York State threatened banded sunfish (*Enneacanthus obesus*) inhabit rivers, lakes, and ponds along the Atlantic coast. Because the banded sunfish are voracious predators of mosquito larvae, they provide a biologically efficient means of controlling the mosquito population. Previous population assessments completed in Zeke's Pond and the Peconic River have suggested that the fish populations are at risk of declining. In order to formulate a plan to promote the growth of the species, a distribution study of sunfish was performed in Zeke's Pond, the Peconic River, and the Peconic River Drainage. The study began by observing and identifying the aquatic vegetation in each pond along with documenting the location of each pond with a Global Positioning System (GPS) unit. The next step was to seine and dip net in areas identified with vegetation favored by the banded sunfish. The fish and predatory species obtained were then measured, documented, and released. A rubric was devised to evaluate the correlation between the banded sunfishes' distribution and the aquatic vegetation present in the seined areas. A total of 27 bodies of water have been studied obtaining 321 individuals of various predatory species. Of the 27 waterways, 12 bodies of water yielded 329 banded sunfish. Results of the distribution survey indicate a correlation between the banded sunfish and ponds with a higher density of bladderwort, white water lilies, and smartweed. Of the sites surveyed by this team, results revealed banded sunfish to be present in all of the ponds listed on the New York State Department of Environmental Conservation's (DEC's) historic banded sunfish sites. This distribution survey was part of a larger ongoing survey that is being conducted by the DEC in preparation for developing a recovery plan for this species.

A characterization of N status in *Populus trichocarpa* inoculated with an endophytic bacteria

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Producing biomass for energy that does not negatively impact food supply will require the establishment of biofuel species on poor quality soils that are not used for agriculture. The association of endophytic bacteria with their plant hosts has been shown to have a growth-

promoting effect for many different plant species and suggests that plant-endophyte interactions may allow improved growth on these marginal soils. However, few relationships between plants and these endophytes have been characterized and studied in detail. Previously, the endophytic bacteria enterobacter 638 was shown to promote growth in *Populus trichocarpa* (poplar). We grew poplar cuttings in Hoagland's solution and investigated the impact of enterobacter on the N status of poplar. To account for possible differences in growth rate, we selected leaves for harvest and analysis using the leaf plastochron index (LPI). In the youngest leaves (LPI 2), nitrate levels were significantly and markedly (120%) higher in poplars inoculated with enterobacter suggesting that these plants were better able to take up nitrate. Free amino acid content and starch content was not altered by the presence of enterobacter, but leaf protein content was reduced by ca. 10%. These data provide preliminary evidence that poplar inoculated with enterobacter may have an improved ability to acquire and assimilate nitrate. This trait would be desirable for feedstock species suitable for growth on marginal soils and suggests that biofuel species may be successfully cultivated on poor quality soils that are not normally suitable for agriculture.

Characterization of Research and Development Laboratory Spaces for Metal Contaminants

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Metals such as antimony, arsenic, beryllium, cadmium, chromium, cobalt, lead and nickel are known for irritating the skin and eyes and, when inhaled, may be very hazardous. Mindful of these dangers, the Brookhaven National Laboratory (BNL) Environmental Safety and Health (ES&H) directorate has a characterization plan for these metal contaminants in surface dust under way in laboratories that are now using or have previously used these metals. As part of this continuing study, we collected air and wipe samples for possible metal contamination. The results were then reviewed for compliance with BNL's guidance levels and regulatory standards. Using the Chemical Management System database, we strategically chose high and low probability locations within a building that would provide a comprehensive analysis of the room. The air sampling pumps were calibrated to 2.5 L/m and sampled for four hours using closed-faced PVC filters. In addition, surface samples were taken using pre-moistened Ghost Wipes in an area of 100 cm². The results were analyzed and compared to applicable Occupational Safety and Health Administration and Department of Energy regulatory standards, American Conference of Governmental Industrial Hygienists guidance levels, and BNL's own Acceptable Surface Contamination level. The contaminant's source was determined through investigating historical usage at the site. Based on our final report, laboratories that show elevated levels are to be reviewed with the ES&H coordinators and specific corrective procedures are to be determined in cooperation with the BNL Industrial Hygiene Department.

*** Vanadium Reduction by *Clostridium***

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Vanadium, found in carbon deposits, is one of the major contaminants in groundwater. Its excessive mobility also allows it to infiltrate the surrounding soil, later to be taken up by plants. Anaerobic bacterium of the Genus *Clostridium*, with known bioremediation capabilities was tested for its potential use in remediating vanadium. After growing the bacteria in a glucose based medium for about 18 hours, the culture was inoculated with vanadium(V). The *Clostridium* oxidized the glucose and transferred the electron to vanadium(V), reducing it to vanadium(IV) and possibly lower oxidation states as well. After 28 hours, only 7.6% of the original concentration of vanadium(V) remained in solution while 26.5% remained in the control containing dead bacteria. The amount of vanadium(IV) in solution fluctuated throughout the experiment, but remained at zero in the controls. This data suggests that much of the vanadium had been absorbed by the bacteria, but without further testing it is impossible to tell how much of the vanadium(V) had actually been reduced to vanadium(IV) or other lower oxidation states. Once further research is done on this method it can become an efficient and cost effective way to remove vanadium from groundwater and prevent it from contaminating the surrounding environment.

Preservation of Fluorescence in Transmission Electron Microscopy for Protein Localization

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The Department of Energy (DOE) faces the challenge of finding new efficient strategies for bioremediating toxic substances in the subsurface at over 5700 sites of contamination. One possible method is a microbial approach involving the sulfate reducing anaerobic bacterium *Desulfovibrio vulgaris Hildenborough* (DvH). DvH is important for its ability to reduce heavy metals such as uranium from its soluble state to an insoluble state thus confining it in the subsurface. Early attempts at using DvH to bioremediate contaminated sites demonstrated the lack of understanding of how a bacterium functions within a microbial community. This prompted the DOE to address bioremediation with a systems biology approach. Part of this approach is characterizing and understanding individual proteins and protein complexes as they function within DvH under normal and stressed conditions. In situ protein localization is a desirable method for the characterization of individual proteins as they function within the cell. A commonly used method to visualize individual proteins and track them inside a cell is fluorescent proteins and correlative microscopy. As fluorescent proteins require oxygen to function properly they are not suited for DvH, therefore we employed a novel tag based labeling technology called SNAP-Cell (Covalys Biosciences AG, Witterswil, Switzerland). The SNAP-Cell system has been widely used in eukaryotic systems and aerobic bacteria, however it has not been used in anaerobic bacteria. In order to proceed to correlative microscopy based protein localization studies, it was necessary to investigate whether the photostable SNAP-Cell fluorophore BG-505 would withstand transmission electron microscopy (TEM) processing. To determine whether the intensity of BG-505 maintained fluorescence throughout TEM processing, measurements were taken after each chemical treatment. The fluorescence intensity data was obtained by averaging nine individual fluorescent cells per treatment. The overall conclusion of the data was that the fluorescence of the BG-505 fluorophore decreased during the fixation step, but was maintained at a detectable level and was therefore preserved throughout processing. Using this fluorophore and SNAP-Cell system, protein localization can proceed through correlative microscopy methods.

Measuring Airflow through Commercial Building HVAC Systems Using Air Velocity Sensors

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In order to prevent buildup of indoor air contaminants within commercial buildings while avoiding excessive use of energy, it is necessary to monitor and control the flow of outdoor air into a building. Currently there are no accurate and economically feasible ways of measuring air intake flow rates in real time, and so many buildings are over-ventilated or under-ventilated. To solve this problem, a method of measuring outdoor air flow into a building that can become widespread is necessary. This study evaluated the accuracy of measuring the air intake flow rate when electronic velocity sensors were installed inside or at the down stream face of air intake louver systems. Louver systems are routinely used in buildings to limit water entry into the building during periods of rain or snow. In the study, a system was created capable of holding different louvers and measuring the flow of air through them, and velocity sensors were inserted in different configurations within the system. The study results indicate that this measurement approach can be reasonably accurate, with typical errors less than 10%, whether the sensors are placed inside the louver or at its outlet. Results also indicated that few sensors are required and calibrations are not necessary at the building site, making it a practical method of measurement for widespread use. Further study is needed to evaluate whether the high accuracy is maintained over time and the acceptability of system hardware and installation costs.

Determining a Relationship Between Standing Water Area and Amphibian Population and Diversity in a Constructed Wetland

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The vital ecosystems of natural wetlands in the United States have often been destroyed. In 1990, Argonne National Laboratory began to build the Advanced Photon Source (APS) and several wetlands were destroyed in the process. In order to comply with the Clean Water Act and the policy of "no net loss," Wetland R was constructed to the south of the APS facility. The health and progress of Wetland R was monitored from 1992 to 1996 and yearly since 2002. In 2006 an amphibian survey was completed. The purpose of this research was to determine if a correlation exists between the area of the standing water and the amphibian population size and diversity. This potential relationship was determined through the use of a weekly timed catch using a dip net, to determine the species diversity. Also, a timed walk

around the wetland was used to determine the number of amphibians sighted per minute, thereby estimating the population size. In addition to data collected in 2008, data from the 2006 study were included to determine correlation coefficients between the standing water area and the species diversity, calculating a value of 0.880; and the standing water area and population size, finding a value of 0.066. This shows no strong positive linear correlation between the standing water area and population size and species diversity, as was claimed by the 2006 study. It is not clear if major differences in precipitation, humidity, and temperature patterns within the data collection period might have changed the results. Further studies should be completed to determine if these findings are influenced by predation patterns or weather-related variables.

A Comparison and Contrast of the Surface Energy Balance at Lamont, Oklahoma During the Summers of 2006 and 2007

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The objective of this project was to analyze the differences in surface energy balance between the summers of 2006 and 2007 at the Lamont, Oklahoma Southern Great Plains (SGP) Atmospheric Radiation Measurement (ARM) Climate Research Facility (ACRF). The Oklahoma summer months of June, July and August of each year were analyzed. This project utilized solar radiation, surface energy flux and surface meteorological data collected at the SGP site and downloaded from the ARM online data archive to illuminate the differences between these two contrasting summers. Daily, monthly and seasonal plots of this data were created and examined. Closure of the surface energy balance and also correlation between the surface fluxes and net radiation was calculated. Analysis of these two summers showed differences in the number of weather events, the amount of precipitation, latent and sensible heat flux, net solar radiation, closure, and strength of correlation between various fluxes. The conclusion of this project was that the summer of 2006 received more solar energy than summer 2007, that average closure of the surface energy balance was better in summer 2007, and that there were significant correlations between the surface fluxes and net radiation during both summers. A greater understanding of the surface energy balance at the SGP ACRF site was obtained, which can be used to guide future research and further the understanding of the surface energy balance at other locations. It is suggested that a longer span of time be analyzed at Lamont, Oklahoma.

Climate Change Effects on Leaf Gene Expression of *Avena barbata* in a Californian Grassland Ecosystem

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Global climate changes are impacting the environmental conditions of many ecosystems. In order to develop an informed understanding of the effects of climatic changes on a grassland ecosystem, a study was conducted to examine plant response to altered rainfall pattern and increased nitrogen availability. *Avena barbata*, an abundant species in many Californian annual grasslands, was grown on natural soil in a climate-controlled greenhouse and submitted to three precipitation treatments (low, ambient and high rainfall), two vegetation types (mixed communities and *A. barbata* monocultures) and two levels of nitrogen in the soil (ambient and addition of NH_4NO_3). Samples were collected from the leaves of *A. barbata* during the reproductive stage, and the mRNA transcript abundance of six genes that play a role in carbon or nitrogen metabolism (RbcS, GS1, GS2, AGPS, Nia, Fd-GOGAT) were studied using real-time polymerase chain reaction (RT-PCR). This study showed that these genes respond differently to varying environmental conditions. Vegetation type had the most significant effect on RNA yield; monocultures yielded significantly more RNA content. The addition of NH_4NO_3 solution was thought to increase the amount of mRNA transcript abundance in RbcS, GS2, and AGPS, but the opposite trend was seen. The results from this study suggest that the developmental stages of the plants and the growth conditions at the time of sampling influence the response of mRNA transcript abundance to changes in environmental conditions. This information on leaf gene expression will be used together with data from soil conditions, root gene expression, microbial activity and other data from this project in a model to predict ecosystem response to climate change.

Home Range and Population Estimation of Red and Gray Foxes at Brookhaven National Laboratory

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As one of few remaining predatory animals in the area, foxes play an important role in Long Island ecosystems; yet little is known about their natural histories there. Non-invasive genetic studies in 2006 and 2007

identified the presence of red foxes (*Vulpes vulpes*) and gray foxes (*Urocyon cinereoargenteus*) at Brookhaven National Laboratory (BNL). A study performed in the summer of 2008 built upon this initial research by investigating the individual home ranges of these fox species and again testing for their presence. Two red fox kits were trapped, one of which was successfully collared and tracked. Additionally, scat was collected for DNA analysis over an eight-week period with a focus on areas with historic gray fox activity. The collared red fox maintained a home range of 0.05 mi^2 but was only tracked for one week before it could no longer be found. It is likely that competition forced the fox out of its parents' home range. Fecal DNA was extracted at a 17% success rate and analyzed using mitochondrial DNA markers. All tested samples were determined to be red foxes. Additionally, no gray foxes were trapped or seen on automated field cameras. This lack of visual and genetic confirmation suggests that there may no longer be a gray fox population at BNL. Sport trapping over the previous winter may have removed the gray foxes that were seen at BNL in the past. Home range data was inconclusive due to difficulties in trapping and collaring a sufficient number of foxes. The problems experienced in finding both red and gray foxes may be evidence of a decrease in both of these populations. Trapping will continue next winter, which, if still unsuccessful, may confirm a population decline.

Water Management in the Hydrogen Polymer Electrolyte Membrane (PEM) Fuel Cells

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The appropriate Relative Humidity (RH) level of the reactant gases inside a fuel cell is required to optimize its electrochemical reaction. The purpose of this research project is to determine the RH levels of the reactants that produce the fuel cell's maximum power output without flooding or drying the membranes. These two extreme conditions must be avoided during operation due to their adverse effect on the catalyst inside the membrane. This research will enable the development of a correlation between the load and the main parameters; namely, reactants RH and temperature. This correlation will be incorporated into the development of a humidity and water management control system which is necessary for the fuel cell to operate optimally at various loading conditions. Accordingly, an experimental setup was built with four humidity and temperature sensors installed on the inlets and outlets of the hydrogen and oxygen and on the five-cell power stack. This system also incorporated two heated humidifiers, one for each reactant gas, to manage the humidity level inside the fuel cell. All humidity and temperature sensors as well as reactant gas flow meters were connected to Lab View software as a data acquisition system. The experimental setup was operated and tested at four relative humidity levels; namely, 60%, 70%, 80%, and 90%. As a result of our experimentation, it is apparent that the optimum relative humidity is 95%. The experimental evidence proves that at this humidity level the fuel cell will have the maximum power output.

The Effect of *Phragmites australis* Invasion on Southern Leopard Frog Tadpole Survival on Long Island

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Phragmites australis is a type of invasive plant whose destructive ecological effects include displacing native species and altering the structure of wetlands. Our research explored the possibility that *P. australis* has a detrimental impact on the survival of the southern leopard frog (*Rana sphenoccephala*) and is a factor in the decline of the frog on Long Island. We raised southern leopard frog tadpoles at six different sites with three different levels of invasion: none, medium, and heavy. The tadpoles were raised in mesh enclosures in situ and their growth and survival was monitored. Basic aspects of water quality were evaluated to determine if the presence of *P. australis* made a notable difference. Results indicate that *P. australis* alone does not have a detrimental impact on tadpole survival, but may be harmful in conjunction with other stress factors such as disease. Water temperature tended to be lower as invasion levels increased, presumably due to an increase in shade. It is possible that the decreased water temperature slows tadpole development. Further research could explore the possibility that *P. australis* does not prevent tadpoles from surviving physically, but affect the adults behaviorally by altering the structure of wetlands. It is possible that sites with heavy *P. australis* invasion are not seen as suitable breeding habitat.

Gravel-Corrected Kd Values for Radionuclides in the Hanford Reservation Pit 30 Area Soils

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The standard measurement of a contaminant's ability to adsorb to sediment is known as the distribution coefficient (Kd), and the coefficient is usually determined by the <2 mm sediment fraction. However, this can mislead adsorption capacity when the gravel fraction is incorporated into the predictive calculation. Radionuclide transport is governed by its ability to adsorb to soil particles affecting a retardation factor (Rf) for the contaminant of interest in relation to the normal movement of groundwater which has an Rf of 1. Kd directly influences Rf. In this experiment, different gravel fractions (0, 10, 30, 50, 80 and 100% gravel) were prepared from Pit 30-2 and 30-3 of the Hanford Site in southeastern Washington State using synthetic groundwater spiked with ⁹⁹Tc, ²³⁷Np and ²³⁸U. The Kd<2 mm and Kd>2 mm values were measured and then gravel-corrections were calculated using two equations: one for Kd,gc,gc=0 where the gravel was simply assumed to be diluted Kd<2 mm and another for Kd,gc,gc=x where Kd,tot was a composite of both Kd<2 mm and Kd>2 mm. Neptunium-237 had a lower sorption capacity than ²³⁸U, and ⁹⁹Tc did not sorb on any fractions. The Kd,gc,gc=0 for ²³⁸U underestimated Kd,tot by 37% and Kd,gc,gc=x underestimated Kd,tot by 5%. The gravel fractions had an adsorptive capacity, significantly less than Kd<2 mm, but larger than Kd,gc,gc=0 which assumed no reactive sorbent. The Kd,gc,gc=x was the best measurement of Kd,tot for ²³⁸U. However, because the ²³⁸U Kd can be significantly influenced by several other factors, this empirically developed gravel correction equation should be used carefully to predict ²³⁸U Kd.

Research on the Effects of Dioxin on the Hepatic System

Amy Green (MONROE COUNTY COMMUNITY COLLEGE, MONROE, MI 48161), Margaret Macdonell (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). Dioxin specifically, 2,3,7,8-tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD) is believed to have a number of adverse health effects on people. However, because dioxin testing cannot be performed on humans, researchers must rely on past data on human exposure to dioxin and current observations collected from animal research. This project involves a research team that reviews and evaluates recent articles focused on discovering the effects of dioxin on the human system to assist the U.S. Environmental Protection Agency (EPA) in compiling adequate and reputable research to support the development of health base levels to be provided to the general public. Each member of the research team focuses on a specific endpoint or body system. For example, a specific focus in the current project was to find information on the effects of TCDD on the hepatic system. To find relevant articles, the research team compiled a database of systematic search terms, which were used to conduct online searches on PubMed. The abstracts acquired from these searches were coded according to their level of relevance to the goal of the project. After the full articles of the higher-order abstracts were retrieved, the articles were read and thoroughly evaluated, and the information gathered from the articles was used to build a database of dose-response data to be used by the EPA for plotting and modeling the effects of TCDD in lower doses. The research will continue as more information is collected, which will help expand the database.

Determining the Flowpaths in Partially Saturated Sediment Samples

Kelly Hinkel (UNIVERSITY OF KENTUCKY, LEXINGTON, KY 40502), Melanie Mayes (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). The objective of this study was to determine the relationship between water flowpaths, water content, and particle size in intact, partially saturated sediment core samples collected from the U.S. Department of Energy's (DOE's) Hanford site in Richland, WA. These physical relationships govern the mobility of radionuclides and contaminants in the Hanford subsurface, which is of concern due to the proximity of the Columbia River. The core samples were oriented such that flow was either parallel to (horizontal) or across (vertical) sedimentary beds. In 2008, the cores were injected with a dye tracer (Brilliant Blue FCF) to identify the flowpaths which contributed to the mobility of these contaminants. We found that in three of the four cores; Vertical Coarse (VC), Vertical Fine (VF) and Horizontal Fine (HF), dissolved dye tracer eluted from the cores, which provided the transport time for the dye to move through the cores. Dye transport times were delayed compared to nonreactive tracers, which was consistent with batch isotherm experiments showing chemical reactivity of the dye with the sediments. Four cores were photographed and dissected into approximately 100 samples as a function of sedimentary layering.

Each core and subsample was carefully collected and weighed. In the horizontal core, in which flow was parallel to bedding, we were able to see that flowpaths followed certain sedimentary layers and avoided others. In contrast, in the vertical cores in which flow crossed beds, the dye spread across entire layers. This was surprising because much of the pore space was occupied by air rather than water. Each sample was dried for 24 hours and weighed again to determine the mass wetness. From this information, the water content and bulk density of each core was determined. From selected samples, particle size analysis (PSA) was conducted using the bouyous hydrometer method to determine the percent of sand, silt, and clay within each sedimentary layer. From the PSA, we determined that VF and HF cores had a much higher percentage of clays than the VC cores. The distribution of mass wetness and the percent of fines were expected to be key components in determining the flowpaths. The flowpaths were all observed to be different due to the orientation of the cores, indicating that flow may isolate into specific sedimentary layers under unsaturated conditions. This information will be used to determine the mobility of the contaminants with respect to the Columbia River.

* Improved Pre-Treatment Process for Mercury Stabilization

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The Sulfur Polymer Stabilization/Solidification (SPSS) process, developed by Brookhaven National Laboratory (BNL) to effectively treat high concentrations of mercury contaminant waste, has been licensed to Newmont Mining Corporation, the largest gold mining company in the world. SPSS uses sulfur polymer cement and other reagents such as NaHS to treat mercury. This process is highly effective; however, testing by BNL and Newmont has found inconsistent leaching results that have been attributed to the presence of small quantities of unreacted mercury. The technical challenge was to design an improved SPSS process in which HgS is formed more effectively without leaving unreacted Hg that is susceptible to leaching. We proposed to improve the SPSS process by introducing a fluidized bed pre-treatment stage. We hypothesized that the reaction from Hg to HgS is predominantly a gas phase, and that reacting gaseous Hg with S powder with high surface area and rapid mixing will more effectively convert Hg to HgS and ultimately result in reduced Hg leaching from SPSS treated waste. We tested the application with a commercial fluidized bed dryer and an experimental fluidized bed column; however, the rapid accumulation of pressure in both test conditions prevents the generation of a sufficient quantity of mercury vapor from developing quickly enough to make this process efficient and cost-effective. We look forward to assembling a more efficient setup to improve the result.

A Brief Evaluation of Common Methods for Extraction and Analysis of Technetium-99 in Contaminated Soil

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Technetium-99 (Tc-99) is a contaminant of interest at numerous nuclear facilities because it is mobile in subsurface environments and is a key contributor to long-term risk. Therefore, the proper quantification of Tc-99 is important for scientists at the Hanford Site in Richland, WA who deal with legacy waste from plutonium production that occurred during World War II and the Cold War era. This study investigated the relative accuracy of three common methods for extracting Tc-99 from contaminated sediment; water extraction, acid extraction and microwave-assisted digestion. A lab-prepared control sample containing a known amount of Tc-99 and 25 sediment samples from the Hanford Site were extracted using these three methods. Half of the filtrate from each extraction was immediately analyzed for Tc-99 content by inductively coupled plasma mass spectrometry (ICP-MS). The other half was treated with TEVA® resin (Eichrom Technologies, LLC) prior to analysis. Microwave digestion of the contaminated sediment samples consistently produced higher results than water and acid extraction. In the case of the untreated control sample, water extraction only recovered 70% of the Tc-99 in the sample and acid extraction recovered 90%, while microwave digestion of the sediment gave average recoveries of 120%. Upon treatment of the samples using TEVA® resin, analysis by microwave digestion became more accurate; recoveries of Tc-99 from the laboratory control samples averaged 102%, whereas the recoveries for water and acid extraction remained at 70% and 90%, respectively. These results indicate that microwave-assisted digestion followed by TEVA® resin treatment is the most appropriate extraction technique to fully quantify Tc-99 concentrations in sediments.

Quantifying the Infectious Period of Bean Leaf Beetles and the Latent Period of Bean Pod Mottle Virus in Soybean

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Bean pod mottle virus (BPMV) can greatly impact soybean yields, with infections that occur early in the season causing the greatest yield losses. The bean leaf beetle (BLB) is the primary insect vector for BPMV, but little is known about the length of time that the beetles remain infectious. In addition, there is scant information on the temporal and spatial dynamics of BPMV within soybean plants. Information on how long it takes from inoculation until a plant is infectious, i.e., time from inoculation to the time that the beetles can feed and acquire the virus, remains unknown. To quantify the infectious period of the BLB, 35 beetles were swept from grass borders near woodlots and allowed to feed on BPMV-infected plants for 48 hours. Individual plastic cages were used to house one beetle per plant and beetles were allowed a transmission period of 24 hours. This process was repeated until the 15th day, where upon beetles were collected and tested for the presence of BPMV using Enzyme-linked immunosorbent assay (ELISA). Following a 21-day incubation period, the sap from each plant that the beetles had fed on was extracted and tested for BPMV using ELISA. To determine the time needed for BPMV to become systemic throughout soybean plants, two sets of 225 plants were mechanically inoculated at the V2 and V5 growth stages. Following inoculation, 25 plants were destructively sampled each day and all leaves from each plant were individually extracted and tested for BPMV using ELISA. To determine if all leaf positions became infected with BPMV following inoculation, 25 plants inoculated at the V2 growth stage were allowed to grow for one month, and all leaves and branches of each plant were individually sampled, sap extracted, and tested for BPMV. The acquisition efficiency for beetles to acquire the virus was 54.3%, but just three of 19 beetles tested positive for BPMV at the end of the study. These results indicate that more than one day is necessary for the beetles to effectively acquire and transmit the virus. The percentage of BLB transmitting BPMV increased from day one (19.4%) to day three (25%). An average of 72.2% of the leaves from each BPMV-inoculated plant tested positive for BPMV 25 days after inoculation. In the V2 and V5 growth stage experiment, the youngest leaves on plants had the highest percentage of leaves testing positive for BPMV five to seven days after inoculation.

Development of Non-Precious Nano-Catalysts for a Proton Exchange Membrane Fuel Cell

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While a fuel cell, especially the Proton Exchange Membrane (PEM), is expected to be an important source of clean energy, the major hindrance for commercialization is its high cost and lack of durability. The Platinum (Pt) catalyst is the most expensive component in a PEM fuel cell system; consequently, extensive efforts are currently underway to reduce the amount of Pt or replace Pt with non-precious nano-materials while maintaining or improving stability, durability, and performance. In this project we have focused on nano-metal catalysts of four different non-precious metals. Nano-metal particles of Nickel (Ni), Cobalt (Co), Copper (Cu), and Silver (Ag) were separately mixed in an ultrasonic bath with Vulcan XC72R carbon black as a catalyst support. Nafion was added to the mix as a binder. Each catalyst mix was prepared with a metal loading to catalyst support of 30% by weight. The electrochemical characterization for each catalytic mixed compound was studied by cyclic voltammetry using a rotating disk electrode. All nanoparticles showed a very small charge in the hydride region for hydrogen oxidation reaction. For oxygen reduction reaction (ORR) the nanoparticles produced a potential of around 0.0 to 0.2 volts. Similar analysis was conducted on these metal catalysts after submerging them for 48 hours in liquid ammonia (NH₃). NH₃-submerged nano-metal particles of Ni, Co, Cu, and Ag resulted in no charge in the hydride region and did not produce any potential for ORR.

Uranium Extraction from Ores the Green Way

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Extraction of uranium from naturally occurring ores is gaining renewed interest because of the worldwide increase in demand for uranium and the recent increase in the cost of petroleum fuels. In this study, we examined the use of citric acid, a cheaper and more environmentally friendly method to extract uranium than the current method. In this process, we mixed various concentrations of citric acid with uranium samples and, after analysis, compared the level of extraction for each concentration of citric acid. We used uranium ores obtained from

Moab, Utah and Cigar Lake, Canada. The ore samples were ground to <0.2 mm and analyzed for uranium content using a Spectrophotometric method. Micro-X-ray Absorption Near Edge Structure analyses at Brookhaven National Laboratory's National Synchrotron Light Source confirmed that uranium was present in hexavalent form in the Moab ore and in tetravalent form in the Cigar Lake mineral. Elemental mapping was done to determine the association of iron, manganese, calcium and other metals with the uranium. X-ray diffraction, done at Stony Brook University, showed that the Moab uranium was composed of silicon oxide and calcium carbonate. The results of this study will be useful for the optimum extraction from both low and high-grade ores. The most efficient concentration for uranium extraction with both Moab and Cigar Lake uranium was 0.8 M citric acid. The efficiencies in extracting uranium for Moab was 72.5%±0.02%; for Cigar Lake was 16.95%±0.24%; and for Cigar Lake with hydrogen peroxide and 0.8 M citric acid, 35.73%±0.00%. The results show that extraction using citric acid is very efficient in the low-grade uranium, but not as efficient in the high-grade uranium. That is why a repeated trial of 0.8 M citric acid and hydrogen peroxide was added in, so that the high-grade uranium could be oxidized to form uranium in its hexavalent form. In the end, this experiment did find a more environmental friendly method, and additionally, extraction using citric acid produced almost no waste.

Minimizing Optical Variability in Optical Measurements of Particles from Second Hand Tobacco Smoke

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Epidemiological studies show that exposure to Particulate Matter (PM) is linked to increased rates of respiratory disease. Currently, it is difficult to reliably measure the concentration and nature of PM in a universal way. As a result, there is a need to develop an inexpensive miniature device that accurately measures the concentration and content of PM in indoor and outdoor air. Prototype particle samplers have been developed to measure PM. The particle sampler employs the principle of thermophoresis to collect PM. Collected material (gas and PM) is analyzed using spectroscopy and gas chromatography. Due to the multi-step nature of determining particulate matter in the air, there are many possible sources of uncertainty in measurement in these experiments. Historically, these variables have been addressed through redesigning instruments and altering the procedures. Standard pre-tests and post tests of electrical power, baseline absorption, flow rate of the pumps, cleanliness, and accompanying devices (aethelometer) are conducted to minimize error. Despite these efforts, actual data still does not fully correlate with expected data. This summer, experiments were designed to identify and correct sources of random error and/or bias as a result of procedural and/or device malfunction or alteration. The objective this Summer was to determine the sources of random and systematic error in spectrometer data as a result of variables that effect light intensity (I) passing through the heat sinks. This experiment focuses on the effect of chipped quartz heat sink tips. Chipping of the quartz rod reduces light intensity passing through the quartz. However, if the rod is chipped before the Reference Intensity (I₀) measurement is taken, there is likely no change in the absorbance post experiment, as calculated with Beer's Law. However, if the quartz is chipped during the experiment, the Intensity (I) of light will decrease, and thus provide increased absorbance readings. Findings suggest that with each consecutive chip (chip 1, chip 2, chip 3) of the same quartz, the intensity decreases within the ultraviolet light range and the visible light range by a difference of 200–1000 counts of intensity. To remedy this issue, we have ordered "quartz tip caps," that will protect the tip and also prevent accidental PM collection.

The Development and Testing of a Novel Thermodenuder for Internal Combustion Engine Emissions Analysis

Bradley Landgraf (ALLEGHENY COLLEGE, MEADVILLE, PA 16335), Meng-Dawn Cheng (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831).

A thermodenuder is an instrument that removes vapor from an aerosol via heat and diffusive transport, leaving behind solid aerosol particles that can be characterized in terms of particle size, number of particles, and other physicochemical properties. The objective of this study was to examine the effects of temperature on the performance of two thermodenuders, one commercially available from TSI® Inc. and one being developed in-house at ORNL. I compared the performance of the in-house developed thermodenuder (ORNL-TD) to that of the TSI Model 3065 thermodenuder using laboratory-generated aerosol particles. A 1% solution of ammonium sulfate [(NH₄)₂SO₄] was aerosolized by an atomizer, conditioned by removing water vapor in a diffusion dryer, and flowed through a bypass line, the TSI 3065 or the ORNL-TD. Both thermodenuders were operated at each of six temperatures: 25, 50,

100, 130, 160 and 200 °C, in separate experiments. The ammonium sulfate aerosol particles were size-classified by an electrostatic classifier and counted using an ultrafine condensation particle counter. Particle losses were compared between the TSI 3065, ORNL-TD, and the bypass line. Results show that the size distributions of the ammonium sulfate particles did not change over the range from room temperature to 160 °C. Above 160 °C, the peak particle size declined significantly, and the number of particles increased, possibly due to decomposition of the chemical forming smaller particles by nucleation. The TSI thermodenuder had a particle loss of 20% or more depending on the operating temperature. The ORNL-TD had a particle loss of 7% under the same conditions used in experiments with the TSI thermodenuder. These results indicate that the ORNL-TD is a promising technology for analyzing aerosols. Additional tests are expected to support these preliminary findings.

Plant Species Diversity Relative to Surface Water Area in a Mitigation Wetland at Argonne National Laboratory

Melissa Laniosz (UNIVERSITY OF ILLINOIS, URBANA-CHAMPAIGN, CHAMPAIGN, IL 60558), Kirk Lagory (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). When the Advanced Photon Source at Argonne National Laboratory in Illinois was constructed in 1990, 1.8 acres of wetland were destroyed. Because the Clean Water Act mandates a no-net-loss of wetland area, a mitigation wetland, Wetland R, was constructed. Wetland R has been monitored from 1992–1996 and 2002–2008 to determine if its plant diversity is comparable to that of the destroyed wetlands. The purpose of this study was to observe the annual change in plant species distribution, focusing on distribution relative to surface water area. Sampling occurred along 10 linear transects in five randomly located 0.25 m² quadrats per transect. Species name, percent cover, and the presence of standing water were recorded. Wetland status, native status, and the coefficient of conservatism were determined for each species. Three hydrology classes were determined based on species distribution in quadrats relative to the frequency of standing water. This year, 83 species were found, 14 more than last year. Native species increased from 73% to 77%. A non-native plant, *Phalaris arundinacea*, was the most abundant with a mean percent cover of 11.5, almost four times the percent cover from last year. *P. arundinacea* was found equally in quadrats not containing water and those with standing water more than 40% of the time. *Boltonia latissuama*, a native, obligate wetland species, was the second most abundant with a mean percent cover of 7.5. *B. latissuama* was predominantly found in quadrats with standing water more than 40% of the time. Studies on the frequency and distribution of native versus non-native species should continue in Wetland R to ensure the wetland is comparable to those which were destroyed.

Rates and Mechanisms of Radionuclide Fixation by Organo-Polyphosphates.

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Contaminants in radioactive wastewaters disposed of into the Y-12 Security Complex S-3 ponds for 32 years have migrated into the surrounding soil and groundwater. This experiment studied the potential role of organo-polyphosphates for uranium and thorium adsorption and immobilization. Phytate is a naturally occurring polyphosphate produced commercially for its utility as a metal chelating and precipitating agent. Polyphosphates can react with contaminants by adsorption, ion exchange, and/or coprecipitation. Forty small (5–10 g) permeable environmental leaching capsules (PELCAPs) were prepared to contain polyacrylamide, alone or in association with soil and polyphosphates. The PELCAPs were submerged in a contaminated groundwater then repeatedly retrieved and assayed using X-ray fluorescence spectrometry (XRF). Uranium and Thorium levels were compared to levels of other elements (Sr, Rb, Fe, Mn and Zr) which remained relatively constant. The small uptake of U and Th by polyacrylamide alone reflected the diffusion of dissolved ions into the gel. Thorium uptake was initially highest by soil only, but the final values of soil and soil+phytates were relatively similar. Uranium uptake values were initially highest in soil+Na phytate, but uptake was quickly dominated by soil+Ca phytate. Future studies will determine the mechanisms of attenuation and degree of leaching of the contaminant-laden PELCAPs. One-half of the PELCAPs will undergo sequential laboratory extractions to determine rates of ion diffusion by deionized water, weak ionic exchange by dissolved salts, and extraction of adsorbed soil oxides by dilute acid. The other half of the PELCAPs will be submerged in uncontaminated in situ groundwater. PELCAPs will be analyzed to determine which materials maintain radionuclide fixation longest relative to the contaminant uptake. As XRF data are insufficient

to conclude the specific means of attenuation, the additional analytical methods of laboratory extractions and in situ leaching will assist in determining these mechanisms of radionuclide fixation.

Lattice Boltzmann Modeling of Reacting Flows

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The objective of this study is to simulate flow and reactions in a tubular reactor. Tubular reactors are the basic building blocks of many catalytic devices, including those on cars used to reduce emissions of carbon-monoxide (CO) and nitrogen oxide (NO_x). Lattice Boltzmann Methods (LBMs) have been applied to many areas where mesoscopic flows are encountered. Our research focuses on using these methods for heterogeneous chemically reacting flows. Predictive models can be used to optimize tubular reactor designs thus increasing their energy efficiency and reducing operating costs. My summer project was debugging and developing a Fortran 90 LBM program, originally written by Sreekanth Pannala and Srdjan Simunovic at Oak Ridge National Laboratory. I applied the program initially to simulate flow in a pipe with no chemical reactions, and compared the results to analytical solutions for fully developed and developing flows. To verify the approach, I simulated Poiseuille pipe flow with periodic boundary conditions and compared the predicted velocity profile to analytical results published by others. I also simulated Poiseuille pipe flow with inflow and outflow boundary conditions, and analyzed the entry-length effects. Now that the code has been verified for flow in the pipe, the chemistry has been “turned on” to simulate reactions within a tubular reactor. The net result of this research was a working Fortran 90 LBM program that accurately simulates flow in a tubular reactor in two dimensions, although it still has limited capabilities for modeling chemical reactions. The ultimate objective of the research is to develop an efficient flow solving LBM program which can play a crucial role in solving reacting flow problems in energy applications that are important to the Department of Energy and the nation.

Our Environment in Hot Water: A Life Cycle Approach to Comparing Tank and Tankless Water Heaters in California

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Residential water heating is a large source of energy use in California homes. This project took a life cycle approach to comparing tank and tankless water heaters in Northern and Southern California. Information about the life cycle phases was calculated using the European Union's Methodology study for EcoDesign of Energy-using Products (MEEUP) and the National Renewable Energy Laboratory's Life Cycle Inventory (NREL LCI) database. In a unit-to-unit comparison, it was found that tankless water heaters would lessen impacts of water heating by reducing annual energy use by 2800 MJ/year (16% compared to tank), and by reducing global warming emissions by 175 kg CO₂ eqv./year (18% reduction). Overall, the production and combustion of natural gas in the use phase had the largest impact. Total waste, volatile organic compounds (VOCs), polycyclic aromatic hydrocarbons (PAHs), particulate matter and heavy-metals-to-air categories were also affected relatively strongly by manufacturing processes. It was estimated that tankless water heater users would have to use 10 more gallons of hot water a day (an increased usage of approximately 20%) to have the same impact as tank water heater users. The project results suggest that if a higher percentage of Californians used tankless water heaters, environmental impacts caused by water heating would be smaller.

Exploring Global Climate Change Research Portfolios and Evaluations Methods

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The U.S. Strategic plan for responses to potential Global Climate Change includes mitigating emissions from non-energy and energy sources, direct CO₂ capture, and adaptation. Since many Argonne research projects are concerned with increased energy efficiency, a Real Options Analysis model (ROA) was adapted and simplified in order to understand the interaction between the research and the market conditions necessary to assess a value for the research. An example case of residential lighting was developed to project two technology adoption transitions: one going from incandescent bulbs to compact fluorescent bulbs (CFL) and another transition to light emitting diodes (LED). Data were collected through Internet sources on the relative production and operation costs, the variability of the price of electricity, the market size necessary, and adoption rates for the two lighting transitions. A scenario was created using data from California since the state is a leading indicator of environmental and energy changes for the country. The value of the research was explored as a function

of the electricity market characteristics and research characteristics, e.g., time and results. The results showed that the greater the energy price volatility the greater the ROA value. The more elongated the research time, the lower the ROA value. The higher the ROA value the shorter the new technology adoption time. This model could be applied to investigate other research efforts and be extended to include more options and realistic assumptions.

Velocity Models Along 12th Street of the 200 East Area, Hanford Site, Washington

Nicole McMahon (UNIVERSITY OF OKLAHOMA, NORMAN, OK 73019), George V. LaSt (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352). Accurate vadose zone and hydrogeological models are essential for remediation at the Hanford Site. Seismic reflection and refraction techniques have the potential to improve our understanding of the subsurface hydrogeological framework, but lack of velocity information has limited the use of these techniques. Velocity models are needed in order to process seismic data correctly. A 4.6 km transect was identified that incorporates eighteen wells coincident with a seismic reflection survey along 12th Street of the 200 East area of the Hanford Site in Washington State. Borehole data were standardized and a geologic cross-section was constructed to portray the surface structure of geologic formations and subunits. This cross-section was then projected onto the newly acquired (2008) seismic reflection line for special comparison. Three different velocity model approaches were evaluated for processing of the seismic data to better reflect the borehole data. These velocity model approaches used Gardner's Equation relating compressional wave velocity and density to estimate the velocities by facies, analog velocity values for specific stratigraphic units obtained from literature, and by studying the relationship between increasing velocity and depth. Inconsistencies between the three different modeling approaches are thought to arise from differences in density measurement methods, the potential inapplicability of Gardner's Equation, and the scales of the model constructs. The velocity models are quite different and need to be further evaluated during seismic data processing. Another velocity model approach to evaluate would be a combination of the velocity models used in this study. Other improvements may include additional data collection and/or accounting for additional factors.

*** Statistical Variations in Bird Survey Data From 2000 to 2007**

Rachael Millings (STATE UNIVERSITY OF NEW YORK-STONY BROOK, STONY BROOK, NY 11722), Jennifer Higbie (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Since 2000, the Environmental & Waste Management Services (EWMS) Division at Brookhaven National Laboratory (BNL) has conducted monthly bird surveys from March through October using a point-count method. The purpose of these surveys is to identify new species in the area; monitor changes in species populations, as well as changes in parasitic species populations; create accurate habitat models; and evaluate the effect of land management on various species. To accomplish this statistical analysis of the data collected from 2000 through 2007 was performed using Statistix 9, an analytical statistics program. The data were organized into smaller files by year, family, and species. Biodiversity indices were calculated for each year. Next, descriptive statistics files, such as scatter plots and pie charts were created to gain a visual perspective of how the number of birds observed varied with respect to weather and temporal variables, as well as how biodiversity indices varied by year. A one-way analysis of variance (ANOVA) test and/or a Kruskal-Wallis nonparametric ANOVA test was then performed on selected data sets to determine the significance of any variation from the mean. Finally, a Geographical Information System was used to identify any correlation between species population variations and habitat availability. The results showed that the brown-headed cowbird (*Molothrus ater*) and the ovenbird (*Seiurus aurocapillus*) experienced population changes during the 2000–2007 period ($\alpha=0.05$). Both increases and decreases in the total sum of birds and bird species observed with respect to season were determined. ANOVA testing also showed that the diversity of the Biology Fields and Peconic River transects was greater than that of the South and Z-Path transects ($\alpha=0.05$). According to the Pearson correlation test, a strong correlation of 0.6581 exists between the species richness of a transect and vegetation type representing more than 30% of the station area. Using these results, the EWMS division at BNL can make informed management decisions concerning the experimental design of the survey method and the oversight of bird species populations and habitats.

Translocation of Radio-Implanted Eastern Tiger Salamanders (*Ambystoma tigrinum tigrinum*)

Sarah Miloski (STATE UNIVERSITY OF NEW YORK-BROCKPORT, BROCKPORT, NY 11951), Valerie Titus (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). A way to combat degrading upland habitat that surrounds amphibian breeding ponds is the translocation of jeopardized species to other wetlands. Information on movement patterns of translocated individuals is crucial to comprehending the ecology of a species by detecting any adverse effects the translocation has on the individual. This type of knowledge is vital when making management decisions regarding land use. The eastern tiger salamander is a New York state endangered amphibian found on New York's Long Island, although its historic range stretches from Long Island down to northern Florida. This amphibian species is affected by increased urbanization that threatens its breeding habitat which makes it a candidate for translocation to suitable habitat. In an effort to determine the impact of translocation on this species, 11 Eastern tiger salamander juveniles were collected from two different ponds, Pond A and Pond B, and implanted with radio transmitters. This allowed for the tracking of movement patterns after pond emergence. Five individuals from Pond A were translocated to Pond B, while five were returned to Pond A. The individual collected from Pond B was implanted and returned to its collection site. All individuals were tracked for four weeks to determine movement patterns and habitat selection through the recording of vegetation in a plot surrounding the individual's location. Of the five individuals returned to their native pond, three were lost to predation, one died in the field, and one was lost when its signal became untraceable. The greatest distance traveled occurred by the salamanders placed at pond of original collection. Of the translocated individuals, four were preyed on. This indicates that translocated individuals are more susceptible to predation. Translocated individuals at Pond B moved a shorter distance, in comparison to individuals at Pond A. This is indicative of stress and unfamiliarity with the area. Due to a very dry summer, Pond A dried up completely, prompting an early emergence of the salamanders at a smaller size, making these individuals more vulnerable to mortality. Although transience existed at both ponds it appears that eastern tiger salamanders fare better when they are not translocated. With the abiotic and biotic factors at the study sites, more research is necessary to deem translocation a worthy way to manage the eastern tiger salamander population of Long Island.

Investigation of Nitrate Removal from Wetlands Receiving Agricultural Runoff

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Agricultural watersheds typically have excess amounts of nitrate-nitrogen in their drainage. High nitrate-nitrogen concentration in water is an environmental and health concern. Nitrate-nitrogen can act as a contaminant in drinking water and cause eutrophication that can deplete dissolved oxygen concentrations and thus endanger aquatic life. For this study, nontidal freshwater wetlands were tested for the treatment of nitrate-contaminated water. This study sought to identify relationships between laboratory microcosms and a full-scale treatment wetland, examine how nitrate-nitrogen load affects organic carbon production, and determine the relationship between influent load and concentration of nitrate-nitrogen in the microcosms. Results showed that the laboratory microcosms were very efficient in treating nitrate-contaminated water, with a range of 80 to 96 percent removal of nitrate-nitrogen. The laboratory microcosms compared to the field site showed a much higher percent removal at similar loads of nitrate-nitrogen. One potential reason that would explain the discrepancy in removal between the microcosms and the field site would be that the laboratory microcosms acted as an ideal, completely mixed system. Also, the plant biomass of the microcosms is predominantly composed of duckweed (*Lemna valdiviana*), which is not found at the field site. The flora at Ramona Lake is mostly comprised of tule (*Schoenoplectus californicus*). One plant species may have the ability to uptake $\text{NO}_3\text{-N}$ more effectively than another, thus affecting the removal percentage. Dissolved organic carbon results showed no measurable response to increased nitrate-nitrogen loads with consistent results and mean concentrations of 4.16 ± 0.51 mgC/L for Microcosm 1 and 4.08 ± 0.69 mgC/L for Microcosm 2. Total organic carbon results were highly variable and uncorrelated with increases in nitrate-nitrogen load; mean total organic carbon concentrations were 6.33 ± 3.98 and 11.34 ± 6.23 mgC/L for Microcosm 1 and 2 respectively. As expected, the data shows a strong linear relationship between nitrate-nitrogen influent load and concentration, with an r^2 value of 0.91 for both microcosms. We conclude that freshwater nontidal wetlands have the potential to treat agricultural runoff at highly efficient rates; however, further research is

needed to investigate what factors specifically allowed the laboratory reactors to be much more efficient when compared to natural wetlands.

In-Situ Monitoring of Trace Gases in a Non-Urban Environment

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This study describes the integration of a set of trace gas analyzers measuring carbon monoxide (CO), ozone (O₃), sulfur dioxide (SO₂), and nitrogen oxides (nitric oxide (NO), nitrogen dioxide (NO₂), and odd nitrogens (NO_x)) into a single rack to facilitate the study of various air chemistry problems. The first application of this system occurred between July 2, 2007 and August 7, 2007 in Richland, WA. The mixing ratios of all species were lower than in most rural-suburban environments, and strong diurnal patterns were observed. The characteristic anticorrelation between ozone and NO_x was observed. As photochemically-formed ozone depleted surrounding daytime NO_x, NO₂ was being replenished at night with ozone destruction. The highest ozone during these episodes was 45 ppb. The overall average was 15 ppb with readings dipping to near zero at times. This observation is low compared to average daytime summer readings of 60–80 ppb in highly populated and industrialized urban areas in the Pacific Northwest region. Four ozone episodes were observed. Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPPLIT) analysis and prevailing weather conditions both indicated much of the ozone was transported locally or produced in situ. Analysis of SO₂ as a tracer for ozone advection further indicated lack of long-range regional transport of pollutants to Richland. The results of this work could be a useful sample data set to study the historical record of air quality in rural eastern Washington.

*** The Cultivation of *Clostridium acetobutylicum* and *Clostridium pasteurianum* for the Production of Ethanol in a Synthetic Medium**

Claribel Nunez (BROOKLYN COLLEGE, BROOKLYN, NY 11213), **Cleveland Dodge** (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

Due to atmospheric pollution and a need to reduce the release of harmful gases to the ozone layer, there has been ongoing research into alternative fuel sources. Ethanol is a source that can reduce the ground-level formation of ozone layer when added to gasoline. Consequently, the study of efficient ways to produce this alcohol has been of great importance. Therefore, the production of ethanol fermentation by *Clostridium acetobutylicum* and *Clostridium pasteurianum* was investigated. These two bacteria were studied under a four mineral salts medium. The growth of the bacteria in these mediums depended on Mg, Fe, and K. In order to maintain the best cell growth and alcohol production both bacteria needed to be kept in neutral pH and in anaerobic conditions. The mediums were neutralized with 1 N Sodium Hydroxide and placed into 150-ml bottles. The mediums were then sparged with nitrogen, autoclaved, and inoculated. Due to time constraints a proper growth curve of the four mineral salts medium was not obtained. The cultures were growing slowly and so it was difficult to obtain accurate data on the optical density and pressure as the cultures grew. Because of this it was also difficult to obtain accurate data on the pH of each medium as the cultures of *C. acetobutylicum* and *C. pasteurianum* continued to grow. Glucose provided to be a better carbon source for *C. acetobutylicum* and *C. pasteurianum* than glycerol. The cultures grew at a more rapid pace when maintained in glucose. Increasing the amount of salts (such as potassium sulfate) and carbon sources (such as yeast extract) were shown to increase the production of ethanol in both cultures. However, even though ethanol increased in both cultures, *C. pasteurianum* showed the most ethanol production when kept in any of the four mineral salts medium.

CO₂ Emissions from the Conversion of Pasture Grasslands to Switchgrass for Bioenergy Production

John Odackal (NEW YORK UNIVERSITY, NEW YORK, NY 10011), **Julie Jastrow** (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439).

Soil and plant biomass contain roughly 2.7 times more carbon dioxide (CO₂) than the earth's atmosphere. While the earth's terrestrial system is currently a CO₂ sink, local CO₂ sequestration and emission is heavily dependent on land management. The conversion of lands to bioenergy crop fields, an increasingly common practice in the U.S. and global communities, might have a significant impact on global atmospheric CO₂ concentration and global warming. This study examines factors affecting soil respiration, a CO₂ emission source, in a brome pasture grassland site recently converted to a switchgrass field. The study site was prepared for planting by burning and herbiciding a 37-year-old brome field. Three different methods were used to investigate CO₂ emission from the switchgrass field. These different methods were CO₂ flux analysis, Keeling plot analysis, and aggregate analysis.

CO₂ respiration was measured for flux analysis using an infrared gas analyzer. Gas samples for Keeling plot analysis were collected at CO₂ concentrations ranging from 450–800 ppm to disaggregate net soil CO₂ emission into root and microbial CO₂ respiration. Soil samples were collected at depths of 0–5 cm for aggregate structure analysis. The results from CO₂ flux analysis show that the average respiration rate of the brome site was nearly double that of the switchgrass field at one week and five weeks after switchgrass planting (p<0.0002 for both time periods). Comparison of CO₂ emission sources at one week after planting using Keeling Plot analysis showed that while root respiration was significantly lower in the switchgrass field (p<0.0001), both the brome and switchgrass sites had similar microbial respiration rates (p=0.93). Initial aggregate analysis shows no significant difference in aggregate distribution between switchgrass and brome sites. It is possible that in the cleared pasture grassland studied, organic material is not the limiting factor of microbial activity. This suggests that long-term studies contextualized by local limiting factors are needed in order to accurately quantify CO₂ emission from the clearing of some land-types to produce bioenergy crops.

Dynamic Modeling of Earthquake Ruptures

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Geophysicists have invested considerable effort in understanding how earthquake ruptures evolve. It is expected that a better understanding of the evolution of earthquake events could lead to improvements in earthquake prediction. If seismologists can more accurately predict the seismic magnitude, duration and location of earthquake events, infrastructure could be better designed and situated to reduce the risk of human injury and property damage. This poster focuses specifically on the dynamics involved in earthquake ruptures. Tectonic forces around earthquake fault zones create stress and strain on the rocks. The rocks are thereby loaded with energy much like a spring. Once the energy load exceeds the fault yield strength, the rock ruptures, releasing this stored energy to the surrounding geological system. In our work we have applied the elastodynamic equation of motion to model how the energy from an earthquake propagates through a geophysical system. We compared two methods that have been used to dynamically model an actual earthquake that occurred in 2000 in Tottori, Japan. The two methods are the Finite Difference and the Finite Element Method (FEM). This poster provides a short theoretical discussion about our comparison of the two modeling methods. In our study, we used the FEM to model the Tottori earthquake. We constructed a three-dimensional model of the fault using ABAQUS® (FEM). We were then able to modify the boundary conditions, such as friction and pre-stress, in order to explore the impact upon the eventual release of energy from the rupture of the fault. These results were then compared to actual data collected from the Tottori earthquake. The results of modeling efforts, such as ours, provide seismologists with information they can use to better predict the energy and duration of seismic events.

Determining the Structure and Defects of Manganese Oxides Using X-Ray Absorption Spectroscopy

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Since manganese oxides are stable over time, and studies suggest that their biologically and abiotically formed states are distinguishable, they possess the key properties to be useful as biosignatures. Biosignatures are biological indicators of life and may be used to search for extraterrestrial life. Because bacteria form poorly crystallized manganese oxides in nature, we must refine detailed crystal structures before being able to utilize them as biosignatures. After performing X-ray Absorption Spectroscopy (XAS) on various manganese oxides and fitting to a single scattering model with Mn-O and Mn-Mn shells, the Extended X-ray Absorption Fine Structure (EXAFS)-derived fit data was compared to X-Ray Diffraction (XRD)-predicted local structure results. In particular, we were able to explain the significantly lower EXAFS coordination numbers for the O and Mn shells compared to the XRD results. Also, by constraining to XRD parameters for fitting, we found increases in disorder and reduced chi square that indicate defects and that EXAFS is a better representation of the structures. We were able to rank the manganese oxides by ideal structure as predicted by XRD, from the least ideal to the most ideal: small tunnel (pyrolusite, ramsdellite), tunnel (coronadite, cryptomelane), layer (chalcopyrite, lithiophorite, birnessite), to layer/tunnel (todorokite).

* The Biodegradation of Ionic Liquids

Trisha Ramdihal (QUEENSBOROUGH COMMUNITY COLLEGE, BAYSIDE, NY 11364), Dr. Cleveland Dodge (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

Ionic liquids (ILs) are organic salts with melting points below 100 °C. Owing to their attractive properties such as non-volatility, non-flammability, high thermal stability, high conductivity and recyclability, ILs have received considerable attention as environmentally friendlier alternatives to conventional solvents. However, the toxicity of ILs and their fate after entering the environment is not clearly understood. Understanding the effect of the structure of ILs on their biodegradability is important for the success of their large scale application and gives insight into possible waste management procedures for spent ILs. The overall goal of this project is to design ionic liquids that will have a minimum negative impact on the environment. Results in the literature indicate that incorporation of ether, hydroxyl, and ester linkages in the cation of ILs is favorable for biodegradation. Halide salts based on the 1-methylimidazolium cation bearing alkyl, hydroxyalkyl, and ethoxyethyl substituents have been successfully synthesized. The halide salts were converted to phosphate containing ILs. H-1, C-13 and P-31 Nuclear magnetic resonance (NMR) spectra were used to confirm the structures of these compounds. The biodegradation of the ILs is being assessed by incubating a fixed volume in a mineral salt medium with the soil microorganisms. After several dilutions at periodic intervals the fate of the IL will be determined by comparing the NMR spectra of the ILs before and after contact with the microorganisms. Preliminary results for hydroxyalkyl imidazolium bromide ILs indicate that the IL was not degraded by the soil microorganisms. Future work will include investigating the ethoxyethyl and alkyl containing ILs in a similar manner.

Fecal Coliform Analysis of Marine Water Seeps in Dungeness Bay, Washington

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For over 15 years the Dungeness watershed, located on the Olympic Peninsula in Washington State, has experienced a steady decline in water quality due primarily to conversion of forested and farmed lands to residential development. The decline in water quality in the Dungeness River has lead to impaired water quality in the connecting estuary, Dungeness Bay, which has resulted in closure of commercial and recreational shellfish beds. The primary cause for the declining water quality and shellfish bed closures has been an increase in fecal coliform, a bacterial indicator associated with fecal contamination from both humans and other warm-blooded animals. A recent microbial source tracking study in the Dungeness watershed has confirmed the presence of human sources of fecal coliform as a partial source of contamination to the Bay. This project was conducted to collect additional fecal coliform data in areas not currently sampled, to determine if further microbial source tracking work is warranted in the Bay. Water samples from freshwater seeps to the Bay were collected at a low tide during the summer and analyzed for fecal coliform. Levels of fecal coliform found in the seep samples ranged from 52 to 1140 colony forming units (CFU)/100 ml. A majority of these concentrations are above state regulatory levels for bacteria in both fresh and marine waters. Although the actual loading from these seeps may not be significant, i.e., low flow, the relatively high concentration from some of the seeps would indicate further investigation to determine what the source of contamination might be (e.g., failing septic systems, animal sources). The overall goal is improved water quality in the Dungeness watershed, and a return of shellfish harvesting in Dungeness Bay.

The Use of Visual Surveys to Determine Odonate Species and Abundance at Vernal Pools at Brookhaven National Lab

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Dragonflies and damselflies are insects of the order *Odonata*, suborders *Anisoptera* and *Zygoptera*, respectively. In the state of New York there are over 170 known, documented species of odonates of the over 5000 species known worldwide. Odonates play an important role in maintaining the delicate ecosystems of vernal pools and other bodies of water such as marshes, streams, and wetlands. Determining the species present and their abundance at a site can be difficult due to their incredible flight speed, their temperamental habits, and the surrounding weather conditions. Visual surveys are the simplest way to document the species and their abundance. Specific ponds onsite at Brookhaven National Laboratory (BNL) were each surveyed once every five to nine days at the same designated time. The survey was

conducted for a full hour and the odonates present were marked as being present at intervals of ten minutes using a number system that denotes ranges of 1 to 5, 6 to 20, 21 to 100, or 100+ individuals. The study was conducted for ten weeks. The surveys have shown a strong presence of some odonates while others have very weak presence or none at all. The surveys have also shown that at certain ponds overall species abundance was declining at an alarming rate unrelated to flight season; hydroperiod may have had a significant effect on certain Odonate species. Through these surveys to identify all Odonates present at BNL we have added to the Odonate Atlas, an existing study that is identifying all odonates of the United States.

Biofuel Sustainability Analysis Using System Dynamics: Economic Impacts

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The U.S. is pursuing a national strategy of energy independence and climatic protection in which domestic renewable carbon-neutral biofuels will displace 30% of U.S. oil consumption by the mid-21st century, stated by President Bush in a 2007 State of the Union Address. Such fuels, including ethanol and biodiesel, will be produced from biological feed stocks (biomass). The availability of this biomass will hinge on the application of modern scientific and engineering tools to create a highly-integrated biofuel production system. Efforts are underway to identify and develop energy crops ranging from agricultural residues to genetically engineered perennials; to develop biology-based processing methods; and to develop large-scale biorefineries to economically convert biomass into fuels. In addition to advancing the biomass-to-biofuel research and development agenda, policy makers are concurrently defining the correct mix of governmental supports and regulations. Given the volumes of biomass and fuels that must flow to successfully enact a national biomass strategy, policies must encourage large-scale markets to form and expand around a tightly integrated system of farmers, fuel producers and transporters, and markets over the course of decades. In formulating such policies, policy makers must address the complex interactions of social, technical, economic, and environmental factors that bind energy production and use. This project developed a dynamic model to explore the potential consequences associated with the national biomass strategy in terms of agricultural/forestry economics. The principles of sustainability were applied to better understand the projected harvests of biomass for food and fuel. A set of sustainable harvest indicators was used to guide policy and strategic direction as well as monitor performance. This particular model allows the user, among other things, to see the relationship between inelastic demand for fuel and pricing of corn grain, profit maximization practices by the market, and the interaction between grain crops and their residues. The results of this preliminary research show that farmers will be very responsive to grain prices and will alter their crop rotation practices to maximize profits with disregard to agricultural sustainable practices. This preliminary examination demonstrates that as biofuel production increases, there needs to be significant attention toward sustainable farming practices. More research on this subject is planned to follow on with these preliminary results.

Production of Hydrogen Gas from Hydrogen Sulfide

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Concerns over global climate change and the rising instability in oil producing regions of the Middle East have had major impacts on the global energy market. The United States has identified the need to transition from an energy strategy heavily dependent on fossil fuels to a more diversified alternative energy plan, including the use of hydrogen. Hydrogen can be used as a clean, efficient, transportable fuel source, emitting only water vapor as exhaust. However the cost of hydrogen is currently a prohibitive factor in the development of a hydrogen based energy plan. Identifying and developing means of efficient and cost effective hydrogen production is a crucial step in establishing hydrogen as a major energy source. The goal of this research is to test and develop techniques for recovering hydrogen gas from hydrogen sulfide (H₂S) using molten copper as a reactant. H₂S is a byproduct of the petroleum and natural gas refining industry. It is toxic to humans, destructive to industrial catalysts and a pollutant to the environment. This research tested methods for safely and efficiently recovering high purity hydrogen gas by reacting H₂S with molten copper. The experimental design for this research is a scale up of the 2003 proof-of-principle system. Experiments were performed to determine maximum possible flow rates for varying melt sizes, effect of flow rate on purity of hydrogen produced, and effect of impurity gases on the process. Knowledge gained from this research may be instrumental in advancing a hydrogen based energy plan in the United States.

Effects of Aerial Herbicide Application on Hanford's Flora

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Herbicides (primarily Tordon® 22K) were applied aerially to 10599 hectares of shrub-steppe habitat located in the Hanford Site in southeastern Washington. These applications were conducted to control invasive weeds such as knapweed (*Centaurea spp*) and yellow starthistle (*Centaurea solstitialis*). Picloram is the active ingredient in Tordon® 22K. To understand the effects that picloram had on the native species, vegetation surveys were conducted to measure the species richness, canopy cover, and frequency of plants growing in herbicide-treated areas. These sites were compared to adjacent areas with similar species and soil composition. Sampling was stratified by year and soil series. Our results showed a significant difference between the canopy cover of forbs growing in treatment areas compared to control areas ($P < 0.0001$). Forb canopy cover was also influenced by soil type in treatment and non-treatment areas ($P = 0.0255$). Grass canopy cover was not different between herbicide areas and untreated areas. Further analysis indicated that herbicide application for all treatment years decreased the canopy cover of native forbs and that diversity was lowered in the treatment areas.

* Determining the Temperature Dependence of Perfluorocarbon Tracer Release Rates from Permeation Sources

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The Tracer Technology Group at Brookhaven National Laboratory (BNL) performs atmospheric transport studies using perfluorocarbon tracers (PFTs). As part of these studies, the tracers must be released into the atmosphere, outdoors or indoors, and the release rate must be well known. One method of releasing small quantities of PFTs ($\mu\text{L}/\text{min}$ vapor) is through the use of permeation sources. These sources generate small emissions rates through the permeation of a volatile fluid (in this case the PFT) through a membrane. The PFT emission rate can be determined by measuring the PFT weight loss over a time and at a given temperature. Since the sources are used indoors and outdoors, they are subject to widely differing temperatures. The emission rate is temperature dependent and this dependency must be well characterized for the sources to be useful in atmospheric studies. The objective of this research was to measure the emission rates of several PFTs through a silicone membrane and to examine the correlation between the PFT emission rate and temperature. In order to achieve this, sixty permeation sources were produced and placed in constant temperature chambers of 8 °C, 20 °C, 30 °C and 40 °C for a period of two weeks per temperature. These sources were small vials, each filled with one of six different liquid PFT types and capped with a permeable silicone rubber membrane. For each temperature test, the sources were weighed daily using a high precision balance and their weights were recorded on EXCEL spreadsheets. The weight loss of each source was calculated by subtracting the last from the initial weight along a two-week data timeline. Then, the PFT weight losses were plotted as a function of time, and from these slopes, the PFT weight loss rates were obtained. As expected, the results showed that the weight loss rates of the tracers were greatest in the 40 °C temperature chamber since at this higher temperature, the tracers become more volatile and the diffusion is increased. From the relationship between the weight loss rates versus temperature, the equation of a linear least-square relations is the temperature dependency which is used to obtain the rate of PFT release experimental source term for the mega sources at given temperatures.

Carbon Dioxide Induced Density Driven Brine Convection: Enhancement of CO₂ Sequestration

Ka Wai Tse (DIABLO VALLEY COLLEGE, PLEASANT HILL, CA 94523), Timothy J. Kneafsey (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720).

This paper presents a two-part experimental study on Density Driven Convection (DDC), a highly desired fluid flow that can greatly enhance carbon dioxide (CO₂) storage in geological media. The first part of the study investigated the subsurface conditions in which DDC occurs. We conducted a series of tests in which gaseous CO₂ was introduced into a pressure vessel containing brine and a porous medium at moderate temperature and pressure. We studied the effects of porous medium permeability and brine salinity by altering these variables in each test and comparing the resulting rate of CO₂ uptake into the brine. In our tests, we discovered that the rate of CO₂ uptake in brine was phenomenally faster in systems of high permeability, indicating that DDC took place. This is because a more permeable system allowed convective flow to occur more easily. Salinity, on the other hand, had an opposite impact; salt made the brine denser which reduced CO₂

dissolution thus DDC was not as likely to occur. Salt also decreased the solubility of CO₂ which further minimized CO₂ dissolution. In the second part of the experimental study, we conducted similar CO₂-brine tests in a transparent Hele-Shaw Cell, two parallel plates attached on the sides and bottom leaving a small aperture. The Hele Shaw cell was a visualization tool that allowed us to see how DDC developed and observe the different stages in the CO₂ uptake process. Our comprehensive experiment provided a data set against which numerical models can be compared since the processes occur over many size scales.

Determining Commercial Water Usage in California through End Uses: What Is the Current Water Use and Are More Water Savings Available?

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Even though water use in commercial and institutional (CI) sectors involves approximately one fourth of the total water demand in an urban area, CI water uses have received less attention than residential sector use in developing statewide water conservation initiatives. This study examined current CI water use in California to see if there are more water savings available through water-efficient technologies and water-conservation behaviors. Techniques used included reading through professional and academic publications, interviewing experts in water-efficient technologies, and searching through industry reports and unpublished documents. This research found that with the exception of hospitals and hotels, CI subsectors have opportunities to reduce annual water usage beyond the estimates projected in 2003. The average 2008 potential water savings corresponds to over 72% of pre-1992 water use (baseline). Potential additional water savings in 2008 when compared with the estimated water usages in 2003 by Pacific Institute assessment are in the range of 5 to 37%, with 20 to 26% being typical. Within CI sectors there is a wide divergence of how subcategories are defined, because not all water utilities include the same type of subsector. More research and collaborative endeavors will be needed to categorize subsectors specifically for determining water use. Since the current state of information on the end uses of water in CI customers remained vague, this research suggests that building managers make information on water usage more visible and available to everyone. Other research will need to account for climate change, type of buildings that use water, and other CI water uses besides kitchen and bathroom water use.

* Isolation of Anaerobic Bacteria with Better Chromate Remediation Capabilities as Compared to *Shewanella oneidensis* MR-1

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Exposure to hexavalent Chromium, Cr (VI), can lead to adverse health effects such as cancer and genetic mutations. Chromium (Cr) is used for hardening steel and extensively in the coating industry to fight corrosion. For example, all structural aluminum (such as that used in aircrafts) is coated with Cr (VI) based coating. However, due to its high solubility, hexavalent chromium used for the above-mentioned applications tends to solubilize and leads to contamination of underground water. Fortunately, the health hazards associated with Cr (VI) are related to its oxidation state. Whereas Cr (VI) is a health hazard, Cr (III) is an important dietary trace element needed for the maintenance of a healthy heart and sugar metabolism. The health hazards associated with exposure to Cr (VI) have prompted research into methods of cleaning up chromium-contaminated sites. During growth and metabolism, bacteria oxidize organic carbon sources available to them and generate excess electrons which may be transferred to Cr (VI), thus reducing it to the less harmful Cr (III). We have an anaerobic enriched culture (BAC-9) capable of removing soluble chromium. We have also investigated the well-known bioremediating capabilities of anaerobically grown *Shewanella oneidensis* MR-1 as a comparison to the enriched culture BAC-9. In our experiments, we used freshly grown (end of exponential phase), autoclaved (dead bacteria), and autoclaved and depressurized (hydrogen removed) enriched cultures that were prepared in serum bottles. These samples were then inoculated with Cr (VI) solutions such that the total concentration of chromium in each serum bottle was 1mM. The concentration of Cr (VI) was analyzed spectrophotometrically using organic reagent diphenylcarbazide (DPC) and an UV-VIS spectrometer at various time intervals. A baseline for the reduction capabilities of the bacteria *S. oneidensis* MR-1 was generated and compared with that of BAC-9 culture. Cr (VI) concentration was observed to decrease as early as fifteen minutes after the addition of chromium. Hence, these

results show that species constituting this culture have a high potential for use in bioremediation of chromium (VI) contaminated sites.

System Dynamics: Water Use and Crops

Leslie Weeks (BRIGHAM YOUNG UNIVERSITY-IDAHO, REXBURG, ID 83440), Jacob J. Jacobson (IDAHO NATIONAL LABORATORY, IDAHO FALLS, ID 83415). As demand rises for renewable, more environmentally friendly energy sources, there is an increase in demand for biofuel ethanol. In order to meet biofuel production goals set forth by Present Bush's State of the Union Address in 2007, many factors must be evaluated to ensure sustainable, renewable energy. The 2007 Energy Independence and Security Act set production goals for biofuel through 2021 (EISA 2007). As demand for biomass for fuel increases, farmers will have to decide whether to grow crops for biofuel production or for food and feed stocks. This analysis will focus on the biomass feedstock component of the biomass supply system and will examine the effects on farming practices, crop selection, crop production, and yields and how changes will affect water consumption and contamination from field runoff. The analysis of impacts will be done on a regional basis and then on a composite national level. It will also help to identify potential constraints on growth and help mitigate impacts of those constraints. This analysis work will focus on developing the algorithms or functional relationships needed to examine the complex relationship between crop selection, water usage, runoff, fertilizer usage and contamination from runoff. The results will be used to develop a dynamic model to examine the long term effects on water sources due to an increase in growing biomass for ethanol production and due to factors such as crop rotations, fertilizer practices and management strategies. This model showed that increased production of corn in response to ethanol demand will put a significant demand on water and will increase nitrate and phosphate contaminants into runoff from cultivated fields. Farmers, in response to increased prices for corn, will move to a single rotation crop system which has a high demand for fertilizer and water consumption. In addition, current fertilizer application practices tend to over apply fertilizer due to access problems during growing seasons. The results of this modeling demonstrate that changing farming practices in response to biofuel demand may stress water systems that are already stressed and that improved fertilizer practices are needed to reduce contaminated agricultural runoff.

*** Understanding Aerosol-Cloud Interactions From Satellite Data**

Banglun Zheng (CONTRA COSTA COLLEGE, SAN PABLO, CA 94806), Surabi Menon (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). Emissions of greenhouse gases (GHG) and small particles (aerosols), affect global climate. The interaction of aerosols with clouds (indirect effect) can increase cloud fraction (CF) and cloud optical thickness (COT), and can reduce cloud effective radius (Reff) if aerosols increase and cloud water stays the same. Thus cloud reflectivity is enhanced and leads to cooling of the surface. This counteracts GHG effects. The correlation between these variables to aerosol optical thickness (AOT, a measure of the amount of aerosols in an atmospheric column) was studied using satellite Moderate Resolution Imaging Spectroradiometer (MODIS). Retrieved data is used to understand aerosol-cloud interactions in specific regions which have seemingly different characteristics. In this study, the data is filtered such that the AOT value is less than 0.6 (due to possible errors reported by MODIS), Cloud Top Temperature (CTT) is greater than 273K (liquid-phase cloud), and Cloud Top Pressure (CTP) is greater than 640 hPa (low level cloud). In our analyses, we find that clear signals of cloud properties changes to AOT in clean regions. In polluted regions, meteorology usually plays a larger role in the changes of these properties, and obscure signals can be found.

Weather Forecasting for the United States

Brittany Zilnicki (FLORIDA INSTITUTE OF TECHNOLOGY, MELBOURNE, FL 32901), Victor Cassella (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). During the past several months, I have been learning how to forecast the weather. In order to forecast it was necessary to learn how to read MM5 models, regional mesoscale models used for creating weather forecasts and climate projections. I also studied satellite imagery such as infrared and visible imagery, in my case just for the United States. I was also required to write a forecast for the Brookhaven National Laboratory community. The requirements of this forecast assignment was to explain the current conditions, and then summarize the four 12-hour periods that followed. My mentor then evaluated my work forecast for the day as well as my accuracy for the prior day's forecast. These forecasts were then used by the BNL scientists.

General Science

Impact of a Local Disease Spread Mechanism in a Spatial Stochastic Foot and Mouth Disease Model

Andrew Demmert (CORNELL UNIVERSITY, ITHACA, NY 14853), Pam Hullinger (LAWRENCE LIVERMORE NATIONAL LABORATORY, LIVERMORE, CA 94550).

Foot and Mouth Disease (FMD) is a highly infectious disease which poses a threat to agriculture and livestock in the United States. To aid in understanding outbreaks, the Multi-scale Epidemiologic Simulation and Analysis (MESA) model at Lawrence Livermore National Laboratory has been used to simulate outbreaks of FMD. The difficulty in obtaining actual facility locations led to the use of randomly generated facility locations within the model. A new set of facility locations was generated using an algorithm which looked for favorable agricultural traits, and this caused a local clustering of facilities. The effect of this clustering on the simulated outbreaks was analyzed with respect to facilities infected, animals infected and duration of the FMD outbreaks. MESA was parameterized, through literature review, to accommodate a directional local spread which approximated aerosol spread of the FMD virus.

Twenty-one scenarios, each with a county of disease origin and facility type of origin, were chosen to test this local spread method. These scenarios were simulated on both of the facility location sets first without local spread to provide a baseline for comparison and again with local spread. Each simulation consisted of 400 Monte Carlo realizations and was run on a Linux cluster using up to 12 processors. The results were analyzed using T Tests and Quantile-Quantile plots. Without local spread enabled, a total of four scenarios showed a significant ($p < 0.05$) increase in the size of the outbreak, while one showed a decrease. When local spread was enabled, a total of five scenarios were larger and none were smaller. Three of these scenarios showed significance in both comparisons. Overall, 14 of the 21 scenarios showed no significant change when simulated on the newer facility location set both with and without the local spread method. The more realistic facility locations did impact the size of the outbreak in some simulations, but two-thirds of the scenarios showed no significance. As such, local spread impacted only areas where the clustering effect was extreme; mild rearrangement of facility locations caused no difference in the simulated outbreaks. Geostatistical methods need to be applied to the facility locations to determine at what limit clustering becomes an issue for disease control.

Mars: The Search for Life

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The object of this education module is to integrate a week-long Mars curriculum in both a formal and informal classroom setting. This module consists of a series of lesson plans about Mars that concentrates on the NASA Phoenix Mission, the search for subsoil ice water, and the potential for the historical existence of life on Mars. The goal of this research is to convey to middle school students the real-time history that is being created through scientific missions, the importance of space discovery, and how these discoveries affect our world. Using resources from NASA's Astrobiology Institute, Cornell University, the University of Arizona and the American Museum of Natural History, five Mars lessons were developed which focus on the purposes and successes of the Phoenix Mission. Assessments will be accomplished throughout the module and will include creating a sustainable habitable environment, constructing a model of the Phoenix Mars Lander, and utilizing problem solving techniques through experimentation and questioning. This advanced understanding of the Phoenix Mission will provide students with valuable experiences that will facilitate higher order thinking about the possibilities of an existence outside of our own and the importance of interplanetary exploration.

Marine Boundary Layer Cloud Properties as a Function of the El Niño/Southern Oscillation

Andrea Fischer (STATE UNIVERSITY OF NEW YORK-STONY BROOK, STONY BROOK, NY 11790), Michael Jensen (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

Marine boundary layer (MBL) clouds are low-lying clouds that are often found along the eastern boundaries of the world's oceans. These cloud systems are important to the earth's climate due to their impact on the local radiation balance through reflection of a great deal of incoming shortwave radiation without a compensating change in longwave radiation. Despite their importance, these clouds are poorly represented in global climate models and, therefore, a better understanding of their properties is necessary. Through global teleconnections, the El Niño/Southern Oscillation (ENSO) cycle may influence weather and cloud systems throughout the world. This study investigates the correlations between the ENSO cycle and MBL cloud

properties. By partitioning statistics of MBL cloud micro- and macro-physical properties using measures of the strength of the ENSO cycle, it is possible to suggest the impacts of the this cycle on MBL cloud systems around the entire globe. Seven years of MBL cloud properties observed by the Moderate Resolution Imaging Spectroradiometer (MODIS) onboard NASA's Terra and Aqua satellites from five regions where MBL clouds are prominent (California, Peru, Canary, Angola and Australia) were partitioned using the Multivariate ENSO Index. There are a higher percentage of MBL clouds with an effective radius (r_e) greater than $15\text{ }\mu\text{m}$ during the warm phase of ENSO, therefore drizzle is greater during the warm phase of ENSO for all regions. Optical depth (t) and liquid water (lwp) are greater during the cold phase for Angola which differs from the other locations; however, the r_e is greater during the cold phase for all locations. Angola's cloud properties may differ from the other observed locations due to dust from the Sahara desert. Australia and California show a greater diurnal range in t , lwp and r_e between Terra and Aqua observations. Cloud diameter (C_D) is larger during the warm phase for California and the Canary Islands, but other regions show no difference in C_D between warm and cold ENSO phases. Therefore, the relationships between MBL cloud properties and ENSO that vary from region to region may be due to differing amounts of atmospheric subsidence, ENSO related variability in the Hadley circulation, or, perhaps, variability in upper level cloudiness. Since MBL clouds are significant to the earth's climate, investigating the influence of ENSO cycles on MBL cloud properties helps understand these clouds and their role in the global climate.

Enhancing Knowledge Management in the Process Development and Integration Laboratory

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As a national laboratory, the DOE National Renewable Energy Laboratory (NREL) is a leader in scientific research. In particular, the process development and integration laboratory (PDIL) is a recent addition to NREL's National Center for Photovoltaics providing extensive capabilities for research in photovoltaic technologies as well as cell fabrication processes. In a lab with such significant potential for collaboration with industry and research partners, it is imperative that effective knowledge management methods are used for information regarding the capabilities of the PDIL. This paper describes a process for supporting two established media for knowledge management: electronic databases and websites. Specifically, this project involved information collection on the capabilities and techniques, including but not limited to operating parameters, special features and applications, of each tool in the PDIL by interviewing each tool owner. This data collection was performed simultaneously with further development of a FileMaker Pro database to store tool information and related documents for internal reference. The information collected was then refined and organized to also serve as content for the PDIL website for public display later this season. The work completed to develop these areas has potential to increase the ongoing national research in photovoltaic technology by greatly enhancing the ease of access to information about the capabilities of the PDIL by both NREL scientists and outside parties.

Factors Affecting Hydrogen Production and Glycogen Storage in the Non-Heterocystous Cyanobacterium *Plectonema boryanum*

Jared Gerschler (HAMPSHIRE COLLEGE, AMHERST, MA 01002), Michael Huesemann (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352).

Plectonema boryanum is a non-heterocystous cyanobacterium capable of hydrogen production in anaerobic, nitrogen-limited environments. *P. boryanum* produces hydrogen through indirect biophotolysis, accumulating glycogen and subsequently using it for hydrogen production. Factors affecting glycogen storage and hydrogen production were investigated in *P. boryanum*. *P. boryanum* was grown in continuously agitated and illuminated Roux bottles, sparged with air/ CO_2 (99.7%/0.3%) during aerobic periods of photosynthesis, and 100% argon during anaerobic periods of hydrogen production. The effect of culture dilution rate on hydrogen production was explored in a series of semi-continuous bioreactors. Among the range of dilution rates tested (5% day⁻¹, 10% day⁻¹ and 20% day⁻¹), it was determined that dilution rate had a negligible effect on hydrogen production rates. Anaerobic/aerobic cycling time was also investigated for its effect on hydrogen production rate. It was demonstrated that the rate of hydrogen production decreased with each subsequent anaerobic/aerobic cycle, and that hydrogen production rates were better maintained with longer cycles (lasting two days) as opposed to shorter cycles (lasting one day). Finally, since the amount of hydrogen production is related to the magnitude of cellular glycogen storage,

four different types of bioreactors (batch, fed-batch, semi-continuous, continuous) were investigated for their ability to promote glycogen storage. It was determined that the batch and fed-batch reactors were the most effective in accumulating glycogen, while the continuous reactor was the least effective.

Community Resilience and Its Social Ontology: an Examination of Relationships

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The objective of this study was to develop an ontology of various entities (e.g., organizations, institutions and people) associated with community resiliency. This ontology will become a resource for understanding entity relationships. It will also be an information repository which communities may use to identify subject matter experts on community and regional resilience. An ontology using Excel and Protégé was created to describe the connections between various entities. The ontology is based on information collected from open resources. These open resources include internet searches of numerous organizations, institutions and people associated with community resilience, exploration of several documents including reports on resiliency, lists of attendees at conferences, interviews with subject matter experts, and copies of presentations given at conferences. The study has shown that identifying and mapping entities associated with community resiliency leads to a very small network. Therefore, entities dealing with resiliency in general were chosen to establish a larger entity base. Many of the connections between entities are too complex for a single ontology. Therefore, the initial ontology was subdivided, using Excel, into three separate but more simplified ontologies based on specific characteristics. The simplified ontologies, as well as the ontology created in Protégé, allow faster access to each entity by providing a better arrangement and organization of essential and key connections. They also provide a better understanding of the relationships between resiliency-related entities.

Development of Traditional and Interactive Communication Tools in the Neutron Scattering Sciences Division

Joshua Jenkins (MIDDLE TENNESSEE STATE UNIVERSITY, MURFREESBORO, TN 37132), Charlie Horak (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831).

A large and rapidly increasing array of digital media formats has created a need for new ways to display and interact with information. This need is particularly evident in communication between the public and the scientific community, as communication here is vital to the efficient use of available tools and successful applications of research. My study in the Neutron Sciences Directorate focused on improving communication tools used within the lab and when interacting with the general public. Using professional design software like Adobe Photoshop, Adobe InDesign and Adobe Illustrator, I designed and updated materials such as posters, postcards, badges and fact sheets. Another part of my project focused on using Adobe Flash to develop a new web application aimed at creating a highly interactive environment where users can find information about Oak Ridge National Laboratory's High Flux Isotope Reactor (HFIR) and Spallation Neutron Source (SNS). This application includes an interactive instrument layout for each site, information pages for each instrument, a video gallery and 360° virtual tour photos. I considered many factors during the development of this application including accessibility, intuitiveness and load times. For example, I decreased load times by keeping each section of the application separate and loading them dynamically as users make requests. My work in the Communications Department should help bridge the gap between professional scientists and the public by making learning about and exploring different areas of SNS and HFIR an enjoyable experience for all.

Wind Resource Assessment for a Large Lattice Met Tower

Joshua McDaniel (UNIVERSITY OF COLORADO—BOULDER, CO 80301), Robi Robichaud (NATIONAL RENEWABLE ENERGY LABORATORY, GOLDEN, CO 89401). The United States Coast Guard (USCG) in Cape May, New Jersey, is using their 108 m free standing communication tower to collect wind data at four heights to assess their wind resource for potential wind turbine applications. At each height there are three anemometers mounted on extended boom arms to provide as much tower clearance as possible. The tower affects the wind speeds recorded by the anemometer up to five tower diameters out from the center of the tower. For an accurate wind assessment that reflects the free wind speed, the tower impact must be accounted for in the wind data analysis. Five methods were developed for determining one wind speed for each height in attempting to most accurately estimate the free wind

speed. The first method was to determine the mean of all three wind speeds at each level. The other methods include: mean of the two highest wind speeds, mean of the two closest wind speeds, mean of the two windward side wind speeds and the iso-speed plot wind deficit method. The first four methods apply a reasoned approach; however, they do not take into account the towers affects on the wind speed readings. The iso-speed plot wind deficit method accounts for the wind direction in relation to the location of the anemometers and estimates the effect, both accelerating and decelerating, of the tower on wind speed depending on orientation. This method, derived from empirical data from wind tunnel testing, augmented through computational fluid dynamics models, represents the most theoretically sound approach for estimating the free wind speed at each height with a tower of this size.

Modeling Ethno-Religious Violence

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New software and modeling techniques are being developed for intelligence analysts to use to model social science theories. The software used for this model was developed by Pacific Northwest National Laboratory. The software, called Bayesian Analysis of Competing Hypotheses (BACH), builds models based on evidence from social science literature. Analysts associate evidence from the social science literature with hypotheses and events in the models. BACH models allow analysts to evaluate the likelihoods of multiple outcomes as a function of the evidence used. This particular model is centered around ethno-religious violence and the likelihood that a particular ethno-religious group could become violent in the future and to what degree. Social science literature was gathered and studied for evidence, possible events and hypotheses. From the evidence, variables were defined and modeled using Bayesian nets and an outcome hypothesis was determined. Connections of events and probabilities of events causing the state of another event were derived from the social science literature and put into the model as evidence. The likelihoods of the competing hypotheses were updated based on the evidence and incorporated uncertainty assessments. From the model and the social science literature it was found that ethno-religious groups are more likely to become more violent when self-determination is present. Religion and religious grievances alone are not reason enough for a group to have a high-level of violence. Using BACH is a valuable way to model social science. BACH allows an analyst to attach evidence to the model and rate the evidence for relevance and credibility. Analysts can take into account the objectivity and reliability of the evidence used to build a model.

Massive Correlated Data Analysis: Predicting the Future with Numbers

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Many complex systems today rely more on the collection of data than on theoretical models to predict future values. An algorithm based on the techniques of Principal Component Analysis (PCA) for the prediction of future values in a set of correlated data was implemented. The data was expressed in the form of a matrix of delayed sections (of length m) of each time series, and a singular value decomposition was performed on it. The last value of the series was then retrieved, using only some of the singular vectors obtained. The optimization of several of the variables was investigated, most significantly, the number of singular vectors to use in the reconstruction of the data. Using only the leading vector, which exhibits a very low oscillation frequency, gave the best results in terms of the absolute error in the prediction. Using mostly the leading vector gave the best results in the accuracy in the direction (increase or decrease) of the predictions. However, these predictions didn't exhibit much oscillatory behavior, which was observed when using several vectors and could be useful for some applications. The effect of varying the row length m , called the embedding dimension, was also studied. The best results were obtained when $m=N/4$, where N is the total number of data points. Further research could be done on the way to work with several variables simultaneously, on the best strategy to predict more than one value, and on a method to predict error bars with each prediction.

Data Reduction by Correlation-Based Sampling Improves The Accuracy of Support Vector Machine-Based Classification

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Support vector machines (SVMs) are machine learning algorithms that classify data by generating boundaries between the input, or

training, vectors in a way that maximizes the distance between the boundaries partitioning training vectors of different classes. Once these boundaries are established, one can use them to determine the class membership of new data, called test data. SVMs are an attractive method for classification in complex informatics systems because they allow non-linear separation of the data. However, applying SVMs to high-throughput informatics data is computationally expensive for both training and testing. Thus, a technique is needed for down-sampling the training space without degrading the statistical performance of the classifier. A method to down-sample the training set based on correlation is presented and compared to a random down-sampling scheme. The correlation coefficients of the training data were computed and highly correlated row pairs were identified as candidates for removal. The algorithm iteratively eliminated rows and evaluated the SVM performance for both the selective and random reductions performed on three datasets, one from materials informatics and two from bioinformatics. At each iteration, the Ohio State University (OSU) SVM with a radial kernel classified the test data, which was evaluated with a Receiver Operating Characteristic (ROC) curve (the area under this curve gives an overall accuracy measurement). The ROC scores from a selective 50% reduction were greater than the ROC scores from a random 50% reduction by 0.0162, 0.0812 and 0.1229, indicating selectively reduced classifiers are more accurate. Performing a paired statistical test of significance (signed rank test) with the ROC scores achieved randomly versus selectively for each dataset resulted in p-values of less than 0.001. Thus, a reduction of the training set based on correlation values provides a statistically significant improvement in classification compared to a random reduction. Training set reduction based on correlation provides an optimized technique for sampling from large-scale data and will enable SVM training for large-scale datasets.

Young Women in Science Program: Program Coordinator

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It has been recognized that the participation of women in science, technology, engineering and mathematics (STEM) fields is too low both from a perspective of equal opportunity and for meeting the projected need of STEM professionals. A lack of knowledge of STEM careers, low self confidence and a limited number of role models, have contributed to females choosing not to pursue STEM fields. At Pacific Northwest National Laboratory (PNNL), the Young Women in Science Program (YWIS) was designed with the goals of providing excellent local high school girls a chance to gain a better understanding of the careers and opportunities in scientific fields and to increase the number of young women in the science, technology, engineering and mathematics (STEM) pipeline. Each summer approximately 10 young women are nominated, selected and appointed mentors at PNNL. While at PNNL, these young women are immersed in the world of research as well as required enrichment seminars. As the program coordinator of YWIS I was responsible for facilitating the seminars, collecting program deliverables, coordinating presentations and trips and visiting the girls in their labs throughout the summer. Due to the experience as the program coordinator, I will be able to share what I have learned about careers in STEM with my future students and colleagues. I will be able to demonstrate to the girls in my classes that they can have a future in science, no matter what anyone tells them. Based upon a 2007 survey, 33 of the 38 girls who have completed the YWIS program have obtained or are currently pursuing a science or mathematics degree. Three former YWIS participants have been hired by PNNL as either technical interns or as full time staff; 11 have participated in Department of Energy sponsored internship programs at PNNL; three are currently in graduate school in STEM fields, and others are working for technology companies. The YWIS program is meeting its goals and has opened the doors to a future in science for many of the girls who have participated in the program in science and engineering. The YWIS program goals are being met and, based upon feedback from the participants, the YWIS program has positively impacted these women's lives.

Testing the Multiwavelet Representation of Functions

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The multiwavelet transformation of functions is one of the most promising methods for analyzing and performing operations on them. The multiwavelet expansion represents functions in terms of a basis of discontinuous multiwavelet functions, which are nonzero over a unit domain. In particular, representations of the Green's function of operators of partial differential equations, constructed in multiwavelet bases, can be proven, in many cases, to be sparse and nearly diagonal.

Thus, the computational complexity of the application of these operators is linear or nearly linear with respect to the problem size, and so is very attractive as a method of solution. As in the development of any complex software, testing must be done to assure that the transformed function behaves correctly with respect to basic algebraic and calculus operations. This testing is done by creating and inputting a variety of functions into a program, calculating the multiwavelet representation of these functions, applying a number of operators to both the original and transformed functions, and comparing the results, demonstrating that operating on the multiwavelet representation is numerically stable and achieves the required accuracy. Said testing demonstrated that the transformed functions do behave correctly with respect to the algebra and calculus operations tested to a high degree of accuracy. Also, as the tests were scaled to higher numbers of processors, the completion times decreased in a smooth log curve. These results were expected, but in obtaining them, debugging was performed and problems were identified and worked around. Further testing should be performed on functions represented with a higher wavelet order, and testing should generally be done as the code is modified and improved. The Joule program, written by George Fann and Robert Harrison, performs the multiwavelet transformation which is tested. The paper, *Adaptive Solution of Partial Differential Equations in Multiwavelet Bases*, by B. Alpert et al., provides background on multiwavelet transformations.

Materials Science

Crystallographic Structure of Scandium Tungstate Determined through the Method of Powder Diffraction

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The internal structure of a crystalline sample is one of the most basic and fundamental properties of a molecule; knowledge of this arrangement is needed for a detailed analysis of the sample's structure-property relationships. This knowledge is essential in the advancement of material sciences, chemistry and engineering. Scandium tungstates are being studied at Argonne National Laboratory due to the occurrence of negative thermal expansion in these materials. While most materials expand with temperature, a small number do not. These materials are of great interest for potential engineering applications for resistance to cracking & weathering. A new phase of scandium tungstate was recently discovered that can be synthesized only at high pressures, but the composition, structure and properties of this phase are yet to be determined. The goal over the course of this internship is to elucidate the structure of this novel phase. To address this, an initial understanding of crystallography and powder diffraction was developed. Secondly, the operation of a synchrotron powder diffraction beamline by the Advanced Photon Source was studied as a method of obtaining data to determine the crystallographic structure of solid state inorganic materials. Data on similar classes of materials was collected to learn how the scientific apparatus is used. Finally, an analysis of previously-collected diffraction data on the target solid state inorganic material, scandium tungstate, was performed using computer programs such as General Structure Analysis System (GSAS) and Experiment Editor Graphical User Interface (EXPGUI). The results of this study will yield a clear molecular picture, complete with symmetry and locations of the atoms comprising this new scandium tungstate phase.

Investigation into Metal Oxide Materials and the Potential for Future Thermoelectric Applications

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Successful thermoelectric (TE) materials are those that combine good electrical conductivity and a high Seebeck coefficient with low thermal conductivity. In general, a TE power circuit or thermopile consists of an n-type and a p-type conductor. The TE power circuit generates a voltage in a temperature gradient. The goal of this project was to determine if an experimental material displayed good electrical and poor thermal conductivities and a good Seebeck coefficient. The figure-of-merit, which varies with temperature, incorporates the Seebeck coefficient, the electrical conductivity and the total thermal conductivity of the material into equation form. Achieving a high figure-of-merit in thermoelectrics is very desirable. Specifically, a single-phase copper aluminate material (CuAlO_2) was formed by using the solid-state method or Pechini method. Gold fibers were oriented onto a cast of CuAlO_2 using material composite theory, leading to the TE measurements. Results of the analysis showed that electrical conductivity and the Seebeck coefficient were not favorable with the new composite material in comparison to previously reported data on CuAlO_2 itself. The new composite material displayed an electrical conductivity that was two magnitudes lower than that of CuAlO_2 alone.

The Seebeck coefficient for the new composite reflected a significantly higher value than its counterpart and indicated that lower-charge carriers are available for the new composite.

The Effect of Additives on Bulk Heterojunction Morphology in Inverted Organic Photovoltaic Devices

Sarah Braden (NORTHWESTERN UNIVERSITY, EVANSTON, IL 60208), Dana Olson (NATIONAL RENEWABLE ENERGY LABORATORY, GOLDEN, CO 89401). Recent studies show that the addition of ~1–3 vol% of 1,8 octanedithiol and 1,8 dibromooctane into an active layer solution for traditional organic photovoltaic devices (OPVs) leads to increased device performance. It is possible that the additives allow for enhanced polymer crystallization (aggregation and ordering) and thereby change the morphology of the bulk heterojunction. The additives also decrease the drying time of the active layer films significantly and do not require subsequent thermal annealing processes. The additives therefore present an advantage in terms of manufacturing, providing an alternative to slow-drying and thermal annealing. This study examined the affects of two additives on both traditional and ZnO inverted device structures. Ultraviolet-visible absorption spectra and current-voltage curves were measured in order to characterize the effects on photovoltaic device performance. Results showed an increase in performance in traditional devices similar to that of other groups, although not of the same magnitude, as well as significant increases in performance for ZnO inverted devices. However, differences between the two additives became apparent within the ZnO inverted device data sets, leading us to believe that the chemical properties, not just the physical parameters, of the additives also play a role in improving device performance.

Characterization of Amorphous Arsenic Triselenide Doped with Iodine for Semiconductor Applications

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Arsenic triselenide (As_2Se_3), a technologically significant infrared transparent amorphous semiconductor, has a room temperature resistivity of $1.012 \times 10^{12} \text{ } \Omega\text{-cm}$. The optical activation energy of As_2Se_3 is 0.85 eV and the band gap, E_g , is 1.51 eV. The high resistivity is an indication of poor charge carrier transport properties, which limit its use for electronic applications. Compositional and processing modifications were made to As_2Se_3 in an effort to improve its charge carrier transport properties. The material was doped with hydrogen to passivate dangling bonds and reduce the density of trapping sites in the material. Additionally, iodine was added to As_2Se_3 to modify the chemical bond structure for increased electron mobility and conductivity. Samples were produced containing 0.5, 1.0 and 5.0 mol% iodine. The electrical properties of the specimens were characterized by measuring current-voltage curves and conductivity as a function of temperature. The physical characteristics of the specimens were characterized by density measurements and X-ray diffraction. Optical properties of the specimens were characterized using Fourier Transform Infrared (FTIR) Spectroscopy and UV-VIS-NIR (ultraviolet, visible and near infrared range) spectroscopy. The effects of hydrogen doping and iodine additions on these properties are presented.

Anode Supported Inorganic Oxide Electrolytes for Use in Proton Exchange Membrane Fuel Cells

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The possibility for a solid-state inorganic oxide based membrane-electrode assembly (MEA) that eliminates the need for the use of sulfonated tetrafluorethylene copolymers, such as Nafion®, typically used in MEAs for Proton Exchange Membrane Fuel Cells (PEMFC) was investigated. To avoid the necessity of controlled water content in polymer membranes, an all solid state MEA is preferable. As a proof of concept, an inorganic oxide, Lithium Nickel Tungsten Oxide (LiNiWO), to be used as a proton conducting membrane, was deposited as a thin film, via sputtering, on an anode support. The anode support was assembled with activated carbon for gas diffusion, graphite for electrical contact, Pt catalyst and Polyvinylidene Fluoride (PVDF) as a binder. The functionality of this anode support for this purpose was optimized, as well as the integration of this assembly into an already functional fuel cell. An anode support with excellent structural integrity, smooth surface and capable of generating a voltage 6% greater than that of the standard cell was developed. A thin film of a few hundred nanometers was deposited successfully, but could not generate a voltage in a fuel cell. Based on subsequent tests, this appeared to be due to the failure of the thin film itself, and not the fuel cell setup or anode support. Though the concept could not be proven, a foundation has been laid out for testing future thin films with the development of the anode support.

The Thermal Stability of Amorphous Indium-Gallium-Zinc-Oxide and Indium-Zinc-Oxide Transparent Conducting Oxides

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Amorphous Indium-Zinc-Oxide (a-IZO) is a transparent conducting oxide (TCO) that displays high conductivity and mobility. Due to its amorphous nature, it has the potential to be roll-to-roll processed, decreasing costs in optoelectronic applications such as photovoltaics. Persistent thermal activation of conductivity change has been observed in a-IZO when heated at temperatures as low as 120 °C. Amorphous Indium-Gallium-Zinc-Oxide (a-IGZO) has been used as a stable active channel layer with low conductivity (10–5 S/cm) in thin-film transistors (TFTs). The stability of these a-IGZO films as compared to a-IZO films is the subject of this study. Films were RF sputtered in a single target sputtering system on glass. The films were characterized before and after annealing for thickness and optical and structural properties. Four-point probe conductivity measurements were taken while the samples were annealed on a ceramic heater in the dark. An aging test measured a-IGZO films conductivity over time and after exposure to light. The persistent thermally activated conductivity change was replicated for a-IZO. In contrast, the a-IGZO films displayed both reversible and semi-reversible conductivity change upon annealing. The thermal conductivity change appeared to have a complex dependence on the details of the film deposition. The film's conductivity was stable in ambient, dark conditions over the period of one week, however resistive films became more resistive after exposure to light. Assuming oxygen vacancies act as the primary carriers in these materials, the reversible conductivity change observed indicates that gallium ions appear to stabilize resistive films to some degree. Thus, a-IZO is better suited for conductive applications while a-IGZO is better suited for semi-conductive applications.

Non-Destructive Inspection of Automotive Spot Welds Using Infrared Imaging

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Spot welding is a form of resistance welding which uses electrodes to pass current through two or more layers of metals in order to melt and join them at a single point. Because of its high efficiency in energy use, spot welding is used extensively in the automotive industry where the process has almost been fully automated by robotic technology. Though these spot welds can be created consistently through constant monitoring, defective spot welds must still be inspected manually by pry-check in order to verify the overall quality of the product. The current inspection process is high cost, low efficiency and labor intensive. The purpose of this research is to investigate ways in which this task can be reliably automated such that poor quality spot welds can be differentiated from good quality spot welds by computers and robotics, thereby reducing production time and costs. This research deals specifically with the thermal conductivity of a spot weld, using an infrared camera to quantify the amount of heat that is transferred from one side of the spot weld to the other in a given time. We hypothesized that the thermal conductivity could be correlated to the quality, thereby allowing us to distinguish between poor and good quality welds. Several different heating and cooling methods were tested in order to determine which would result in the most potential for automation and consistency. By taking the data and creating a model, a reliable system may be created in order to assure that an automated quality check using the information obtained can produce an accuracy rate similar or better than that of destructive inspection. A flash lamp and heat gun were each used as heating methods, while cold water, ice cubes, cold air and volatile liquid were used as cooling methods. The resulting data was compared to determine which method, if any, was able to create a series of data curves which allowed good and poor quality spot welds to be differentiated. We determined that a method that could create the greatest temperature difference in the shortest amount of time was more likely to result in data that showed differentiation between good and bad spot welds. The volatile liquid, specifically difluoroethane from a commercial gas duster, showed the most promise for consistent results and easy automation. Future work will consist of creating an easily automated and consistent system which could be integrated into an automotive production line.

Precise Fabrication of Optical Nanoantennas for Novel Applications

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Optical antennas are one of the most exciting contributions from the

field of plasmonics to near field microscopy, providing the ability to investigate the optical properties of matter on previously unprecedented length scales. Based on a novel nanofabrication method presented in this paper, it is now possible to produce and place optical antennas that couple plasmons to the visible regime of light. With this method a mask resembling the optical antenna is deposited on a 20 nm Au substrate via E-Beam Deposition and subsequently etched using Argon dry etching techniques to produce the optical antennas out of Au. Dark field measurements were used to characterize the bowtie antennas. Initial findings show promising results, with well-defined antennas being fabricated with a high degree of accuracy. Antennas with gap sizes in the ~10 nm range have been produced, with minor inconsistencies in the structures edges and surrounding materials due to varying deposition and etch times. Fabrication of single antennas directly to Atomic Force Microscope tips has also been achieved. Additionally, we have taken spectrograph readings that show the antennas producing relatively high intensity light in the visible regime. With further research into the intricacies of the fabrication process, these optical antennas should provide a new method of near field microscopy.

Viscoelastic Properties of Alcell Lignin for Carbon Fiber Production

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Incorporating carbon fiber into automobiles will decrease vehicle weight, thereby increasing fuel economy and decreasing carbon dioxide (CO₂) emissions. However, the current means of producing carbon fiber from petroleum resources is expensive, which prohibits the large scale application of carbon fiber in vehicles. Lignin, the second most abundant organic material on earth after cellulose, is an inexpensive and renewable alternative to traditional precursor materials for carbon fiber production. For example, Alcell,™ lignin, a by-product of cellulosic ethanol production, is attractive as a possible precursor for producing carbon fiber for automobiles. However, substantial research is necessary to identify process conditions for precursor fiber production and subsequent processing into carbon fiber. This project explores the rheological properties of Alcell lignin, which are important for understanding its physical behavior during the melting and spinning of the material into fibers. Complex viscosity and moduli data were collected by means of a rheometer, using Dynamic Frequency, Strain and Time Sweep tests at four specified temperatures (150, 160, 170 and 180 °C) and in two atmospheric environments (nitrogen and air). The information that was gathered displays the environment and temperature conditions at which Alcell lignin exhibits physical characteristics most suitable for subsequent production of carbon fibers. Complex viscosity data collected from each test indicate the ideal temperature range for successful continuous spinning of a precursor fiber to be between 150 °C and 170 °C. In addition, consistent viscosity behavior in Dynamic Strain and Frequency tests show the sample's resemblance to a Newtonian fluid. Therefore, Alcell fibers can be spun at a higher flow rate without sacrificing fiber consistency, a favorable finding that could lead to higher manufacturing yields.

Exploring Indentation Size Effects in Amorphous Metal

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Size effects on mechanical behavior are of scientific interest because current continuum plasticity theories generally do not incorporate microstructural length scales. Size effects have received considerable attention in crystalline metals, but relatively little in amorphous metals. The objective of this experiment is to increase the understanding of size effects in mechanical tests on an amorphous metal called BAM 11, which has the composition $Zr_{52.5}Al_{10}Ti_5Cu_{17.5}Ni_{14.5}$. Nanoindentation tests on this Zr-based amorphous metal provide insights into size effects by using different tip radii. There is a second objective to these experiments: to see if shear bands can introduce microstructural length scales that cause size effects similar to dislocation-related size effects. BAM 11 is prepared by arc casting it into a cylindrical shape and cutting it into smaller samples using an electric discharge machine. The samples are then compressed using a hydraulic MTS testing machine to different pre-strain values. The samples are mounted in epoxy and ground and polished for the nanoindentation tests. The results are analyzed to obtain shear stress values. The load-displacement curves from the nanoindentation tests did not always show clear pop-ins, which are sharp shifts in displacement with relatively small load change. A possible explanation for pop-ins in crystalline metals is nucleation of dislocations and the change from elastic to plastic deformation. In amorphous metals pop-ins are thought to indicate the nucleation of shear bands. When pop-ins did not occur, a curve with a clear

pop-in was used as a reference for determining the onset of plastic deformation by deviation from the elastic portion of the curve. The average shear stresses needed to initiate plasticity show no significant size effect for the as-cast amorphous metal. However, a size effect is seen when internal length scales are introduced into the samples by pre-straining them prior to indentation. Similar size effects are seen in crystalline metals which contain an internal length scale related to the mean free path between dislocations. The size effect reported here, which is based on the stress to initiate plasticity, is different from the conventional indentation size effect, which is based on hardness and therefore includes both initial yielding plus work hardening.

Characteristics of the Biocompatibility of Polymerized 1-Decyl-3-vinylimidazolium Chloride-Based Materials

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Responsive, soft ionic liquid material may be useful for its electronic and optical properties as materials and eventually in devices that can be controlled by external stimuli, such as temperature, light and solvent conditions. Testing the characteristics of biocompatibility of ionic liquid materials is necessary when considering potential uses for such devices and the safety of persons who come in contact with the devices, whether during manufacturing or in use. To measure the effect of ionic liquid materials on the Chinese Hamsters Ovary (CHO) cells, the cells were cultured with the polymerized ionic liquids (PILs). We ran each assay simultaneously under four different conditions: with complete F-12 Kaign's Modification (cF12KM) media alone, with cF12KM and PILs, with cF12KM and PILs with gold nanoparticles and with cF12KM containing varying concentrations of phenol. The biocompatibility assays were evaluated using both dye exclusion and a colorimetric test. We used Trypan blue viability dye to assess the membrane integrity of the cells after overnight exposure; and we used a metabolic 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-2H-tetrazolium bromide (MTT) assay, a standard assay to determine cell viability and cytotoxicity, to assess cellular metabolic activity after overnight exposure. We found that the poly-1-decyl-3-vinylimidazolium (poly[C10VIm]⁺[Cl⁻]) and poly[C10VIm]⁺[Cl⁻] with gold nanoparticles have no adverse effects on CHO cell viability and cytotoxicity.

Evaluation of Inconel 617 and Haynes 230 for Gen IV Nuclear Reactor Application

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Two super alloys, Inconel 617 (617) and Haynes 230 (230), currently are under consideration as candidate structural materials for applications in the Generation IV Nuclear Reactor (Gen IV) Systems. The manufacturers of these alloys have been competing rigorously for several years, trying to establish that their alloy is more suitable for use in the reactor project. The primary objective of this study was to clarify which alloy would be a more suitable material for use in the Gen IV application. A secondary objective was to determine the effect of product forms, if any, on mechanical properties of the two alloys. Creep test data were prepared and input in the Gen IV Materials Handbook database, and some Handbook internal functionalities were used to facilitate analyses of creep resistance. The analyses include sorting data and plotting curves of creep rupture stress versus the time at various temperatures, for each alloy. The two data sets then were used to compare creep rupture resistance of the alloys, and to develop distinctive predictions on the lifespan of each alloy under specified service conditions. In addition, Larson-Miller analyses, $P=(T+460)(\log t+20) \times 10^3$, was conducted to predict the material behavior after very long periods that are beyond practical possible testing times. I found that the creep strength of 617 and 230 plates were similar for temperatures of 760 and 871 °C. Further, bars of 230 showed slightly less creep strength than bars of 617. However this trend was stronger for both alloys at temperatures of 760 to 982 °C. Using Larson-Miller Analyses, 617 and 230 plates proved similar, but 617 was noticeably stronger in the lower stress range. Applying the same analysis to bars of 617 and 230 yielded similar results; 230 were slightly weaker throughout the temperature range tested. After completing my research, I conclude that alloys 617 and 230 are virtually equivalent in terms of creep resistance. Minor distinctions were apparent between different product forms, but these differences were not significant enough to conclude that one alloy is more suitable than the other, for use in a reactor. Additional tests are necessary on other properties such as environmental resistance, radiation effects, fracture toughness, microstructure stability and weldability to determine which alloy should be used in the Gen IV Nuclear Reactor Systems.

Solvothermal Synthesis of Metal Phosphides and Phosphates

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Solvothermal synthesis is a low temperature hydrothermal crystal growth method. The objective of this research was to explore the metal phosphides and phosphates which could be produced by solvothermal synthesis. Metal phosphides and phosphates are of interest because of such diverse physical behaviors as superconductivity, low dimensional magnetism and enhanced thermopower. Lower temperature synthesis is advantageous for energy efficiency, but in the context of this study it was also important because the lower temperatures could allow for the stabilization of metastable phases. FactSage, a chemical thermodynamics database system, was used to determine possible phase equilibria. From this it was determined that phosphides are stable under lower eH/pH and phosphates are stable over a broad range of pH at higher eH conditions. Red phosphorous and the metals or metal salts were combined with water in Teflon-lined Parr autoclaves. The autoclaves were then placed in a furnace for approximately 20 hours at 225 °C. Phase identification and relative phase abundance were determined using a PANalytical X-ray powder diffractometer. The magnetic susceptibility of selected samples was measured between 2 and 350K using a Quantum Design Physical Properties Measurement System. This research focused on the synthesis of cobalt phosphates (e.g., $\text{Co}_2(\text{P}_{207}) \cdot 2\text{H}_2\text{O}$) and nickel phosphides (e.g., Ni_{12}P_5) but other binary and ternary metal phosphides were also attempted. In the case of $\text{Co}_2(\text{P}_{207}) \cdot 2\text{H}_2\text{O}$, magnetic susceptibility screening showed a sharp antiferromagnetic ordering transition at 11K. A temperature dependent neutron powder diffraction experiment is in progress using both the deuterated and hydrogenous forms of $\text{Co}_2(\text{P}_{207}) \cdot 2\text{H}_2\text{O}$ to determine the magnetic structure. Analysis of the neutron diffraction data will provide the magnetic moments and orientation of the cobalt ions in the lattice. It was demonstrated that solvothermal synthesis is an effective method to explore the synthesis and phase relations of a wide range of metastable and high temperature metal phosphides and metal phosphates.

Accelerated Wear Testing of Ultrananocrystalline Diamond-Coated Pump Seals

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The performance of industrial chemical pumps can depend directly on the performance of the seals installed within the pumps. Using a chemical vapor deposition process developed at Argonne National Laboratory, scientists can coat standard pump seals with a thin layer of Ultrananocrystalline Diamond (UNCD™). Prior laboratory tests conducted at Argonne found that when subjected to identical conditions as uncoated seals, UNCD™-coated seals show increased energy efficiency and dramatically increased seal life expectancy. The objective of the experiment was to design a system that can be used to verify these findings by subjecting UNCD™-coated and uncoated seals to accelerated wear conditions. The experimental protocol required the pumping of an abrasive slurry of diatomaceous earth for 100 consecutive hours. Prior to their installation into the abrasive pump testing system, Raman spectroscopy and surface profilometry was used to analyze and characterize the surfaces of uncoated and UNCD™-coated seals. Before performing a complete 100 hour test with both identical pumps, the system was evaluated for robustness and durability using only the pump containing the uncoated seal. Critical temperatures, pressures and flows were continuously recorded while abrasives were pumped for 100 hours. Upon completion of the test, components of the test system were inspected for damage due to the abrasives. Accelerated wear was found on system parts, requiring design modifications to the experimental system. Analysis was performed on the uncoated seal. Wear on this seal was evaluated by comparison between pre and post-experimental surface profile analyses. When system modifications are complete, both UNCD™-coated and uncoated seals will be subjected to identical accelerated wear conditions. Wear on the seals will be compared using surface profilometry and Raman spectroscopy.

Development of High-Efficiency Thermoelectric Material P-Type Filled Skutterudite $\text{CeFe}_4\text{Sb}_{12}$ for Vehicle Waste Heat Utilization

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Thermoelectric (TE) devices based on thermoelectric materials can convert heat directly into electricity without hazardous emissions or can use electricity for cooling without chlorofluorocarbons (CFCs). In order for a thermoelectric device to have high efficiency, both n-type and p-type thermoelectric materials with a comparable high figure of merit, ZT (a parameter characterizing the performance of thermoelectric

materials) is needed. Filled skutterudite compounds have been proven to be promising new thermoelectric materials for waste heat recovery. Currently, the ZT value of n-type filled skutterudite reaches 1.3 at about 800K while the highest ZT of p-type filled skutterudite is less than 1 at the same temperature. To enhance the ZT value of p-type filled skutterudite compounds, a new synthesis technique which combines melt spinning and Spark Plasma Sintering (SPS) was used to produce the p-type filled skutterudite $\text{CeFe}_4\text{Sb}_{12}$. The phase composition was confirmed using X-ray powder diffraction. Transport property measurements were performed to obtain the electrical resistivity, thermal conductivity and Seebeck coefficient on a physical property measurement system (PPMS). Our new synthesis process produced a filled skutterudite $\text{CeFe}_4\text{Sb}_{12}$ with superior thermoelectric properties. The electrical resistivity of our samples is much lower than that previously published, while the Seebeck coefficient and thermal conductivity values are comparable with previous data resulting in more than 20% enhancement of the ZT value at room temperature. This study demonstrates that our new synthesis is very promising route toward producing highly efficient thermoelectric materials.

Cure Characterization of Bisphenol E Cyanate Ester-Zirconium Tungstate Composites

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Zirconium tungstate (ZrW_{208}) is a ceramic material characterized by strongly negative isotropic thermal expansion over a wide temperature range. Several studies have shown that ZrW_{208} reinforcement can improve the dimensional stability of a composite by decreasing the overall coefficient of thermal expansion (CTE). However, the influence of ZrW_{208} reinforcements on the cure behavior of the resin has not yet been examined. In this work, the cure behavior of a bisphenol E cyanate ester (BECy) resin with a ZrW_{208} filler is characterized by differential scanning calorimetry (DSC). The impact of the negative CTE filler on the composite glass transition temperature (T_g) and thermal stability are also investigated. Furthermore, because thermal properties of composites have been shown to be influenced by surface functionalization of filler particles, the effect of silane-functionalized ZrW_{208} on cure behavior and overall thermal properties is examined. The ability of phenomenological reaction models to describe the cure behavior observed by dynamic DSC measurements is tested, and kinetic parameters determined by model calculations are used to predict the isothermal cure behavior of the resin.

Minimizing Temperature Errors in High Temperature Powder X-Ray Diffraction

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X-ray diffraction data may incorporate significant systematic instrumental errors that compromise the calculation of the crystal lattice parameters. One of the major challenges to collecting accurate X-ray diffraction data on samples at high temperatures is accurate knowledge of the sample temperature. The existence of temperature errors is known, but their exact magnitude for high-temperature X-ray diffraction (HTXRD) attachments used at Oak Ridge National Laboratory (ORNL) had not previously been quantified. The objective of this study was to quantify the magnitude of the temperature errors and to test possible methods for reducing them. Standard materials with known thermal expansion were evaluated for calibrating the temperature measurements from 25 °C to 400 °C. Two different high-temperature stages, an Anton-Paar TTK450 and a Bühler HDK 2.3, were characterized and tested with copper and aluminum powder standards on PANalytical X'Pert Pro and Scintag PADX X-ray diffractometers, respectively. Various methods for improving thermal contact of the powders were tested to determine their impact on reducing the margin of sample temperature errors. Analysis of the diffraction scans on copper and aluminum powders yielded precise and accurate crystal lattice parameters at temperatures from 25 °C to 400 °C, and these materials were found to be suitable for temperature calibration standards. When compared to the well-known values of thermal expansion, it was found that the temperature of the powder was significantly less than indicated by the thermocouple. Hence, when running scans in vacuum, per the manufacturer's recommendation, the powder temperature is not the same as the holder. At 400 °C, the difference was approximately 165 °C. Use of DuPont™ Kapton® film as a cover over the powder sample made no difference in the results in vacuum. However, flooding the chamber with helium gas improved thermal contact of the powders, eliminating the temperature gradient between the near-surface sampling volume and the sample holder. The magnitude of the temperature error under several conditions has been

determined. Various strategies to eliminate the error have been tested. The best solution to date has been to flood the chamber with helium gas.

Investigation of Novel Carbon Single-Wall Nanotube Supported Platinum and Platinum-Ruthenium Catalysts for the Oxygen Reduction Reaction in Proton Exchange Membrane Fuel Cells

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Reducing the noble metal loading, most notably platinum, of the cathode in proton exchange membrane fuel cells (PEMFCs) represents the single greatest barrier to reducing the cost of (and thus improving the economic viability of mass production and commercialization of) PEMFCs for transportation purposes. Novel carbon single-wall nanotube (SWNT) supported platinum and platinum-ruthenium catalysts were investigated for their electrochemical and catalytic activity towards the oxygen reduction reaction (ORR). Electrochemical characterization was performed utilizing a standard three electrode cell in which cyclic voltammetry (CV) and rotating disk electrode (RDE) voltammetry measurements were taken. The responses of the SWNT samples were compared to those of a commercial platinum on carbon black material and a synthesized platinum on activated carbon material. Transmission electron microscopy (TEM) was used to determine the metal particle size and dispersion on the SWNT and activated carbon material. Catalytic activity towards the ORR for the SWNT samples was detected in the CVs, however quantitative activity was unable to be determined by RDE measurements due to low platinum/platinum-ruthenium loading on the electrodes (0.9 $\mu\text{g}/\text{cm}^2$). The TEM data revealed small metal particle size of ≈ 5 nm in Pt SWNT and ≈ 3 nm particles in Pt-Ru SWNT. The results of the TEM measurements coupled with larger signal intensity in the CV data suggest increased catalytic activity for the SWNT samples over the Pt/C materials, supporting the utilization of SWNTs as catalyst supports to increase utilization of noble metals and thus decrease total catalyst loading in PEMFCs.

Expanding the XPS Surface Science Spectra Database to Include Hafnium Oxide Thin Films

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In this study, X-ray photoelectron spectroscopy (XPS) characterization was performed on hafnium oxide (HfO_2) thin films grown by atomic layer deposition. HfO_2 is currently being studied to replace silicon oxide (SiO_2) as a gate dielectric in electronic transistors. To help expand scientific knowledge of this material, the datasets collected in this study will be submitted to the American Vacuum Society's Surface Science Spectra (SSS) journal for publication in a peer-reviewed manuscript. This quarterly journal archives spectra of technological and scientific interest, such as those collected in this study. Currently there is limited data on HfO_2 in the SSS database. XPS spectra were collected on a Physical Electronics Quantum 2000 Scanning ESCA Microprobe using a monochromatic Al K α X-ray (1486.6 eV) excitation source. The sample was analyzed under the following conditions: 'as received', after UV irradiation for five minutes, and after sputter cleaning with 2 kV Ar $^+$ ions for 180 seconds. Survey scans showed carbon, oxygen and hafnium as the major species in the film. Carbon initially composed approximately 20% of the surface scanned, but after UV cleaning it was dramatically reduced to 5.1%. This demonstrated that the majority of the carbon was due to surface atmospheric contamination. However, after sputtering there were still traces; this suggests that the carbon left in the film is from precursors used in synthesis. Furthermore, the stoichiometric ratio of oxygen and hafnium confirms the purity of our sample and gives confidence in submitting these to SSS as reference quality spectra. In the future, XPS characterization can be performed for other materials of interest and submitted to SSS so the journal can aid in further surface science research.

The Optimization of Atomic Layer Deposition Parameters for Zinc Oxide and Aluminum-Doped Zinc Oxide Films as Transparent Conducting Oxides in Dye-Sensitized Solar Cells

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Severely low efficiencies have outweighed the benefits of low-cost and the manufacturing ease of dye-sensitized solar cells (DSSCs). However, recent nano-scale developments are unlocking new possibilities and rekindling considerable interest in these solar cells. Novel high-aspect-ratio substrates are being fabricated to support more light-harvesting dye and create a more direct path for electrons in the DSSC photovoltaic circuit, but the enhanced efficiencies are still too low for widespread application. The deposition of thin transparent conducting oxide (TCO) films, such as zinc oxide (ZnO) and

aluminum-doped zinc oxide (AZO), on the surface of these substrates can increase DSSC efficiency by providing a more efficient electron transport. Therefore, the effects of deposition parameters on the optical and electrical properties of thin TCO coatings on high-aspect-ratio substrates need to be studied in order to create an optimal film. This study measured the resistivities and optical transmittances of ZnO and AZO films on anodic aluminum oxide membranes using atomic layer deposition, a thin-film deposition technique involving a binary sequence of self-limiting surface reactions. Spectroscopic ellipsometry, spectrophotometry and four-point probe resistance measurements were used to study the effects of varying oxidizer strengths (H_2O , H_2O_2 and O_3) and deposition temperatures (50–200 °C). Results have confirmed that a weaker oxidizer such as H_2O , as well as a higher deposition temperature, creates a significantly more conductive film. Optical transmittance, however, trends in the opposite direction; stronger oxidizers such as O_3 and deposition at lower temperatures lead to more transparent films. These observations suggest that both deposition temperature and oxidizer strength affect the number of oxygen vacancies in n-type conductive ZnO films. Also, the 5% aluminum AZO films were observed to enhance the conductivity of ZnO without compromising a significant amount of optical transmittance. In conclusion, AZO films are seen as advantageous over ZnO films as TCOs, but the optimal choice of oxidizer and deposition temperature will depend upon the relative influences of conductivity and transparency on the overall efficiency of the DSSC. Further studies on the effects of annealing the films after deposition would be advantageous to a more complete understanding of the potential ZnO and AZO films have as TCOs in nanostructured DSSCs.

Device Optimization for New Scintillator Materials

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The threat of thermonuclear or radiological attack against the United States requires deployment of detection systems to screen for shipments of dangerous radioactive materials. Scintillator detectors for gamma radiation are being developed that provide improved radioisotope identification, in order to identify threat materials within the environmental background of naturally occurring radiation. The highest energy resolution commercial scintillator is Lanthanum Bromide, $\text{LaBr}_3(\text{Ce})$, providing ~2.6% resolution at 662 keV. The goal is to identify materials and device engineering approaches to push energy resolution to ~2%. By analyzing the periodic table and considering materials' properties, single-crystal scintillators such as Strontium Iodide, $\text{SrI}_2(\text{Eu})$ and garnet oxide ceramics are being developed by Lawrence Livermore National Laboratory and its collaborators. The focus has been on device engineering for energy resolution optimization. Considerations include the quantum efficiency (QE) of the photodetector, noise in the photodetector, preamplifier settings and optimization of optical interfaces. Each scintillator material requires different optimization of those parameters. While $\text{SrI}_2(\text{Eu})$ and $\text{LaBr}_3(\text{Ce})$ offer comparable energy resolution, the best photomultiplier tube (PMT) for them is the Hamamatsu 6231 ultrabialkali. It shows a consistently better resolution than a standard Hamamatsu 6231 (2.7% versus 2.9% energy resolution). Cerium-doped garnets emit in the 500–700 nm range, best matched with the Hamamatsu 329EGP PMT. Finally, an avalanche photodiode (APD) detection system was set up, which looks most promising for improving the energy resolution of garnets, due to the high QE of APDs, near 85%. The hope is that these cutting-edge developments will enable the U.S. to have safer and more secure ports and borders.

Atomic Layer Deposition of Alumina on High Surface Area Silica Powders

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Alumina is a transparent insulating oxide which is widely used as a catalyst support layer. Thin films of alumina can be grown by atomic layer deposition (ALD) down to the nanoscale of one monolayer per reaction cycle by using trimethylaluminum and water. The purpose of this project was to determine whether nanoporous silica powders with high surface areas could be uniformly coated with alumina by the ALD method such that full saturation could occur. X-ray fluorescence and direct weight measurements were used to determine the growth rate of alumina with respect to the number of reaction cycles during growth. In order to better understand the surface chemistry of these powders, the properties of the alumina coated powders were analyzed using scanning electron microscopy and energy dispersive analysis of X-rays (EDAX) measurements. These measurements revealed uniform infiltration of the high surface area powder by the ALD alumina coating.

There is future interest in growing cobalt oxide on silica powders by ALD for its potential use as a catalyst in nanoporous membranes using alumina as a support.

Characterization of Cadmium Zinc Telluride Crystals (CZT) and Constructing and Testing a 16 Array Detector

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The key problem of CdZnTe (CZT) crystals is their lack of uniformity since defects or inclusions found in the layers within the crystal itself effect the overall response for a radiation detector. To aid in the selection of the best crystals for a radiation detector, this project employed a tool for analyzing the structural defects of a crystal and then incorporated these crystals into an array detector for further testing to determine the success of the detector. To begin the analysis of the CZT crystals we took infrared (IR) images of the crystals. For an analysis to identify and better understand the defects in each crystal accurately, we employed a three-dimensional virtualization of the crystal using a programming language called Interface Data Language (IDL). After an analysis of the IR images of crystals that provided enough data for a successful examination using IDL, we determined the five best crystals we had to complete a 16 crystal array. This detector array is currently being tested and results are not yet available. This work, an extension of previous research, aims to produce a less expensive radiation detector that exceeds the most robust radiation detectors currently available.

The Analysis of the Chemical Vapor Infiltration Process: Transport Phenomena and Chemical Characterization

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The Chemical Vapor Infiltration process produces high performance ceramic composite materials used in the transportation industry. The process involves the pyrolysis of a gas at high temperatures causing the densification of preforms with various shapes and chemical compositions. This study focused on creating a model capable of incorporating binary and Knudsen diffusion, temperature and pressure gradients and various chemical mechanisms. We tested the model using a carbon-carbon isothermal process with a pressure gradient incorporating a binary homogenous and heterogeneous reaction scheme. The study used the Dusty-Gas Model to incorporate transport processes and a "dominant" scheme for the reaction mechanism. The model was simulated using Finite Difference Method coded in MATLAB. The model output was compared with online Mass Spectrometry on a 9:1 argon-acetylene mixture at 973K with and without a catalyst. The variable parameters introduced in the model were adjusted to fit the experimental data. The model achieved a flow profile consistent with physical intuition. At the first time step the concentration of Argon was given an inverse normal curve, while the concentration of Acetylene could be fit to a normal curve, both due to the pressure gradient. On experimental results, the Acetylene evolved mainly into Butyl-radicals and butane, with lower concentrations of benzene rings. We propose to incorporate a larger set of molecules under transport phenomena given a diverse reaction scheme. Later, we will incorporate the transport phenomena of radical hydrocarbons. Further experimentation will be done to show that the model does describe the densification of the preform within an acceptable tolerance.

Development of Hot Wire Chemical Vapor Deposition for Transparent Conducting Oxides

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The increasing need for alternative energy resources has resulted in a heightened effort for photovoltaic (PV) device research and development. One integral area in many PV technologies is the transparent conducting oxide (TCO) which allows light to pass through it and reach the photo-active layer of the solar cell while acting as a back electrical contact. Current TCO production techniques offer many disadvantages, such as energetic bombardment and high annealing temperatures that may hinder the evolution of PV technologies. A technique called Hot-Wire Chemical Vapor Deposition (HWCVD) promises to eliminate these barriers. This project explores the manufacture of a ZnO dedicated HWCVD system and presents preliminary results of thin film deposition from this chamber. Several materials were attempted for use as filament materials, but most were unable to withstand high temperatures in an oxidizing environment for extended periods of time. Of the materials examined, only iridium was

viable in the required conditions. Many combinations of parameters were attempted before successful deposition of a thin film was obtained. The first TCO produced had a conductivity of 43.9 S/cm and was comprised of 47.62% O, 4.77% Zn and 47.61% Ir. As a response to this film's high iridium content, further experiments were performed with a lower filament temperature to reduce out gassing or oxidation. The second TCO deposited showed an improved composition as a result of this lower filament temperature, at 54.32% O, 28.74% Zn, 9.01% Si and 7.93% Ir. This second film was too thin to obtain conductivity measurements.

Tailoring Better Absorbing Active Material Blends for Organic Photovoltaics

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Solar cells based on organic semiconductor materials are an attractive alternative to conventional inorganic photovoltaics in that they are potentially easier to fabricate at lower cost. Unfortunately, organic photovoltaic devices (OPVs) have low light-to-electricity conversion efficiencies of slightly over 5% — too low to provide cost-competitive electricity. Material factors that limit OPV's efficiencies include insufficient absorption in the broad spectrum of solar light, poor conversion of excitations to electrical charge and poor electrical conductivity. Our research seeks to understand these limiting factors and to develop more efficient solar cells by, for example, improving the active layer absorption or choosing materials with better electrical charge mobility. We first fabricated OPV devices from a 1:1 mixture solution of polythiophene (P3HT), a p-type semiconductor, and a fullerene derivative (PCBM), an n-type semiconductor. This blend absorbs light at wavelengths between 400–650 nm, and has an absorption length (a-1) of 320 nm at wavelength 480 nm. Our best devices yielded efficiencies of 4.3%. We then investigated whether small thiol molecules added to the P3HT:PCBM blend would change the material absorption due to improved morphology. By adding 2.5% 1,8 dithiol molecules, the peak absorption was red-shifted by 40 nm to 520 nm, which is useful as the solar spectrum has more photons at longer-wavelengths. There is also a decrease in a-1 at longer wavelengths specifically a 44% decrease in a-1 at 600 nm. This reduction is important since it allows the absorption of comparable photons with a significantly thinner film. Motivated by this result, we explored novel blends of pentacene (p-type) and perylene (n-type). Since both materials absorb light, this provides additional flexibility in tailoring the absorption of the active material blend. Pentacene also has ~100x better charge mobility than P3HT. We measured the pentacene: perylene blend absorption to be 400–600 nm, and a-1 to be 57 nm at ~545 nm — a significant reduction. The peak absorption is red-shifted by 65 nm compared to P3HT:PCBM and by 25 nm compared to P3HT:PCBM with thiol, again capturing more of the longer wavelength solar spectrum. Having improved the active material's absorption, our next challenge will be to retain the improved absorption while optimizing the other material properties, such as phase separation, morphology and charge mobility, which are required for high-efficiency devices.

Computational Study of Xenon Bubbles in Uranium Dioxide Nuclear Fuel

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There is renewed interest in nuclear energy because of its potential to provide energy without the release of greenhouse gases or carbon emissions that occur when burning coal, a widely used fuel source to date. During reactor operation, fission gas (Xe) bubbles form in nuclear fuel (UO_2) resulting in degradation of the properties of the fuel. The evolution of fission gas bubbles in nuclear fuel has been widely investigated, yet poorly understood. Computer simulations have the potential to shed light on experimentally inaccessible phenomena occurring in fuel under operating conditions. In the present work, molecular dynamics (MD) simulations were performed to investigate the structural changes of Xenon (Xe) bubbles in Uranium Dioxide (UO_2). Two different sized systems were studied; a small cell with ~4000 atoms and a larger cell with ~1.4 million atoms that required use of the MPP2 super computer at Pacific Northwest National Laboratory (PNNL). Xenon was implanted in a face centered cubic (fcc) configuration at the center of the UO_2 cell after removing atoms in a stoichiometric ratio. The smaller system was heated to various temperatures ranging from 300–5000K over a period of time from 2 ps to 0.1 ns. A swift ion track of 3 electron Volts (eV) per atom and radius of 3 nm was implemented in the large system. Smaller systems were also given recoil energy. It was discovered that the heating had minimal effects on the integrity of Xenon clusters. Radiation and recoil energy caused significant distortion of the bubble. Kinetically the large scale

system annealed itself after a few picoseconds. The study suggests that Xenon bubbles in Uranium Dioxide are relatively stable under the limited set of conditions examined in this study.

Surface Chromium Segregation in Iron-Chromium Alloys: A Thermodynamic Approach

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Materials for Generation-IV (Gen-IV) nuclear reactors and the first wall of future fusion engines face severe conditions such as high temperatures, radiation and corrosive environments. Thus, the structural materials used must be immune to such conditions. The radiation and corrosion damage that occurs in ferritic alloys strongly depends on the chromium (Cr) content. In an attempt to understand the physical mechanism behind corrosion resistance in such materials, Cr segregation to the surface of iron-chromium (FeCr) alloys was studied. Out of the three components that determine corrosion behavior, namely, thermodynamic equilibrium factors, migration kinetics and oxygen presence, the thermodynamic factor was studied in this work. A specific Monte Carlo method, the Metropolis algorithm in the transmutation ensemble, was used in conjunction with an accurate interatomic potential for FeCr. Computer simulations captured the complex thermodynamics of the FeCr sample, in particular, the Cr redistribution in the presence of free surfaces. Simulations were carried out at a temperature of 800K in an effort to create the environment that the Gen-IV reactors operate in (~500 °C). The Cr chemical potential was adjusted to get 5, 10, 12, 15, 20 and 35 atomic % (at %) global chromium content. The samples were spheres so that any precipitates or segregation that occurred could be observed in all surface orientations in a single sample. A depletion of Cr at the surface occurred at each composition studied. This depletion occurred for both solid solution and the two-phase region. Precipitates of Cr did not form in the alloy until the Cr content was at or above 15%. The depletion of Cr at the surface suggested that corrosion resistance does not occur in FeCr alloys. Experimentally, FeCr is a corrosion resistant alloy, showing a much enhanced resistance when the Cr content in the alloy is above 15 at %, probably due to the presence of precipitates. The apparent discrepancy between the simulations and the experimental results suggested that the mechanism responsible for Cr segregation may be related to the kinetic effects, overcoming the thermodynamic tendency found in this work. Therefore, it was concluded that segregation is most likely related to kinetic effects that would drive Cr to the surface or to the presence of oxygen. Both effects will be considered in future simulations.

Effect of Hydrogen on the Mechanical Properties of Pipeline Steels

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Due to increasing demands for energy, economies are looking for alternative fuel sources. Hydrogen (H_2) is being considered an alternative fuel; it is renewable, and, in an oxidized form (as H_2O) it is exceedingly abundant. If H_2 became a primary fuel, dependence on foreign sources of fossil fuels would decline dramatically. H_2 , like fossil fuels, will need to be transported from production sites to use sites, probably using pipelines. Studies have shown that H_2 tends to embrittle certain kinds of steels. However, very little information is available on H_2 -caused embrittlement of pipeline steels exposed directly to high-pressure H_2 . The objective of my work is to conduct tensile-strength tests in a high-pressure H_2 atmosphere, and thereby determine the effect of H_2 on the mechanical properties of these steels. This study may yield insights on the best and most cost effective way to transport H_2 through pipelines. I conducted tensile-strength tests on specimens of four types of pipeline steels by placing them in air, hydrogen, or helium atmospheres, and determining changes in the mechanical properties of each specimen. During these tests, an increasing uniaxial force was applied to the specimen and the total time and load applied were monitored continuously until specimen failure. I converted the load-versus-time data from the tests into load-versus-elongation and stress-versus-strain curves to assess tensile strength and other strength characterizations of the materials. The tests used steels of different compositions to compare the effect of H_2 on these steels. The results of the tests show that a H_2 atmosphere reduces the elongation of the material, causing the steels to become more brittle. This, in turn, could increase the risk of pipeline failure when transporting H_2 at high pressures. The tests that I conducted are helpful in identifying steels that are better suited for the high pressure transport of H_2 .

Fabrication of Monovalent Nanoparticles for Site-Specific attachment in Au-DNA Superlattices

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Nanoparticles synthesized with DNA are building blocks with an unexplored molecular versatility that allows them to be considered for a range of applications within the fields of optics, medicine and energy. Due to the programmable and functional nature of DNA, it is readily used as the mechanism for the self-assembly of nanoparticles into crystalline lattices. The repeating unit cells that make up these structures can be manipulated through varying both the nanoparticle and the DNA. A key component of efficient synthesis involves being able to control the amount of DNA per nanoparticle which effects the local connectivity and the overall structural morphology of the aggregate due to changes in the bonding. In particular, monovalent (with one DNA) particles are desired for directed incorporation within the DNA-particle lattice. The goal was to develop a reliable method for the fabrication of monovalent particles, in this case 5 nm gold particles, with controllable recognition properties for their site-specific attachment to DNA in the lattice. However, particles functionalized with only one thiolated DNA are unstable, so the particle surface needed to be coated with phosphane prior to adding the DNA. Overall, current efforts include development of methods for synthesis, purification and characterization using gel electrophoresis, UV-VIS Spectroscopy and dynamic light scattering (DLS). Gel electrophoresis allowed for the separation of bands based on the number of DNA attached to the particle. Placing the desired bands in dialysis tubes within an electric field allowed for the particles to be accessed in order to confirm the number of DNA. The interference from the background in the UV-Vis Spectroscopy characterization data prevented us from confirming the number of DNA on the particle at this time while the DLS data showed that the size of the particle was directly related to the band. However, based on the imprecision of the data, the measurements need to be repeated under different parameters in order to produce a reliable characterization which will reveal the success of the overall fabrication process. Once these monovalent particles can be consistently synthesized, we will be able to fully test their interactions within a crystalline lattice. Through studying the characteristics of these new lattices, we could discover novel magnetic and optic properties that can be applied in areas such as biodetection.

Exploring New Catalyst for High Temperature Polymer Electrolyte Membrane Fuel Cells

Adriana Rico (UNIVERSITY OF NEW MEXICO, ALBUQUERQUE, NM 87101), John B. Kerr (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). New energy technologies, such as vehicles equipped with hydrogen fuel cells, should have the ability to revolutionize and reduce energy use as well as contribute to solutions for the Global Climate Change problem. However, before fuel cell vehicles can reach the mass market, significant research and development must be made to reduce their cost and improve performance. The most substantial cost factor for fuel cells is their dependency on platinum, which is used as the catalyst on both the anode and the cathode electrodes. The goal of this research is to explore possible improved and effective catalysts to be used with a polymer membrane that can withstand high temperatures. Restricting overall power production, splitting oxygen molecules into oxygen atoms, and the subsequent formation of water, is currently the major rate-limiting step in the process of obtaining energy from fuel cells. Novel catalysts would promote a more efficient reaction and therefore remove the cost of using an expensive all-platinum catalyst. In a search for an effective catalyst that would be able to carry out an oxygen reduction reaction, transition-metal ions were combined with various heterocyclic compounds to prepare coordination complexes. Cobalt(II) and Iron(II) complexes of imidazole, bis-imidazole and dipyriddy were synthesized. Using cyclic voltammetry measurements, a comparison of electrochemical properties of each different complex was made, and it was observed that dipyriddy complexes have a better ability to catalyze oxygen reduction reactions. It was also found that complexes with several unoccupied binding sites allow for a faster oxygen reduction reaction because oxygen is able to bind, and in turn, oxidize the metal.

Effect of High-Pressure Torsion on Microstructure Evolution in Nanostructured Materials

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High-Pressure Torsion (HPT), a novel method of metal grain refinement, can reduce industry metal grain sizes by about 1000X from 20–200 μm to about 200 nm. However, when the original grain size is already nanometer-sized, it is unknown how HPT affects a metal's

microstructure. This study was conducted to determine how such small grain-sized metals would react to HPT. The study used high-purity Ni samples with original grain sizes of 20 nm, 100 nm and 1000 nm. These samples were subjected to torsion at levels of 5 GPa and 5 or 10 rotations. The Ni samples, along with reference samples which had not been subjected to torsion (including a coarse-grain sample of 100- μm grain size), were examined using a state-of-the-art small angle neutron scattering (SANS) instrument at ORNL's High Flux Isotope Reactor. The data were reduced and analyzed using Igor Pro software and fit to Guinier models to determine particle sizes. The data also were compared by size and level of torsion to attain qualitative information on microstructure changes with torsion. Surprisingly, under the same torsion conditions, the SANS data for three size classes of Ni samples overlapped, indicating that the eventual microstructure is determined by the torsion deformation, regardless of the initial microstructure. The SANS data showed that torsion causes the loss of small grains as larger grains form, indicating a coarsening behavior. Smaller grain boundaries also were lost as larger boundaries formed. Further work will include modeling the data to extract particle-size distribution as a function of torsion deformation. An examination by ultra-small-angle neutron scattering would be useful in extending this distribution to the actual grain sizes, as well.

Synthesizing and Characterizing TiO_2 and SnO_2 Nanoparticles

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Titanium dioxide (TiO_2) and tin dioxide (SnO_2) have very different electrical properties but similar crystal structures (rutile and cassiterite). We hope that by combining these oxides in individual nanoparticles we can observe their unique structure and functional properties that may be useful in many applications. This project focused on synthesizing and characterizing TiO_2 and SnO_2 nanoparticles in a range of 10–20 nm. In synthesizing these particles, we can study the composition of the nanoparticle surface, determine its effect on the environment, and characterize its aggregation properties. From other studies we can learn whether these particular nanoparticles will be useful in optics, mechanics, air pollution and water waste control. Synthesis was done by using SnCl_4 and TiCl_4 as our metal ion source, benzyl alcohol as the solvent and oxygen source, and CTAB (cetyl trimethyl ammonium bromide) as the surfactant in an Argon gas environment. We characterized our nanoparticles by using X-ray diffraction (XRD), scanning and scanning transmission electron microscopy (SEM and STEM) and other techniques. By analysis of peak width from a database library on the XRD we confirmed that we were successful in making SnO_2 nanoparticles. Using SEM we found that even a small amount (0.5% of solvent weight) of surfactant significantly influenced our particle size. From this we found that SnO_2 nanoparticles can be synthesized under similar conditions as TiO_2 nanoparticles. To complete the project we plan to produce a functional mixed-oxide nanoparticle that may combine the properties of the two pure oxides.

Development of an Accelerated Fiber Length Measurement Method

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Fuel economy of passenger vehicles increases as vehicle weight decreases. Before putting light-weight fiber-based components into production as a way to reduce vehicle weight, it is important to accurately predict how the new materials will handle the various conditions of being a part of a passenger vehicle. But to verify the accuracy of and make adjustments to an engineering property-prediction model of polymer composite structures, data are needed on the structure's fiber length distribution. The objective of this study was to find a faster process of measuring fiber length, by automating repetitive tasks in the current method. To accomplish this, fiber samples were selected from plaques of the target material and prepared using a sample-selection technique developed earlier in the project. Fibers were spread into petri dishes and scanned into a 48-bit color image and two 8-bit grey-scale images. ImageJ, an image-processing application, was chosen as a platform to develop a plug-in to automatically detect, count and measure fibers. To detect the fibers, digital images were pre-processed with a hysteresis threshold. The fibers were counted and measured using a combination of ImageJ's ability to analyze particles in a binary image and a third party plug-in that classifies the particles based on properties such as perimeter, area and average color intensity. The results from a manual counting method were compared to those from the automated counting method; this comparison yielded very similar results from both methods. On a histogram with 0.05 mm bin-widths, the two data sets yielded an R^2 value of 0.94. In each stage (thresholding, analyzing and classifying), the algorithm needs to be

fitted with parameters for the stage to be complete. These parameters, especially those used in the thresholding stage, differ for every image. Therefore, tests are needed to determine what values should be assigned to the parameters in order to optimize performance. Tests also could be conducted to compare the two counting methods in more detail. The method developed here can be used to count fibers more quickly and, with more research, probably more accurately.

Determining the Microstrain of Biological Composites by X-Ray Diffraction

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The mechanical properties of biological composites are often more desirable than those of the material's constituent parts. These emergent properties are determined by the microstructure of the composite and how the material components interact on a microscopic level. In order to better understand how the emergent properties arise, the function of the constituent parts of the material must be known. In this research, the mechanical properties of the biological composite nacre, also known as mother of pearl, were investigated by applying various levels of strain to prepared samples. The microscopic response of the material was observed using X-ray diffraction techniques. Diffraction patterns collected from the nacre samples were analyzed and the full three-dimensional strain tensor was found for each level of applied strain. The Young's modulus of the material in several crystallographic directions was determined from the knowledge of the applied load, sample geometry and measured strain. This information was used to estimate the partitioning of stress in the constituent parts of nacre. It was found that the polymer portion of nacre takes significantly more than its weight percent of the load, which may explain the material's extraordinary toughness.

A Comparison of the Wear of Iron, Nickel and Cobalt-Based Alloys for Use as Exhaust Valves in Heavy Duty Diesel Engines

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Advanced energy efficient diesel engines require increased performance from materials including those used for exhaust valves. One way to make valves more durable is to change their alloy composition. The focus of this study was to compare candidate exhaust valve alloys to see how well they endure when they are subjected to conditions similar to those found in a diesel engine. This comparison was done by running tests on a custom built test machine, the High Temperature Repetitive Impact tester (HTRI). The study looked at how each of the chosen materials responded to the high temperature and oxidation. As well as how the materials held up when subjected to the repetitive impact and sliding to which valve faces and seats are exposed in a heavy duty diesel engine. For this study, three alloys, based on iron, nickel and cobalt, were chosen to give a wide spectrum of material properties common to valves. The results from these tests show that the cobalt-based alloy was better able to resist the wear from the impact and the tangential sliding than the nickel-based alloy. It also better endured the corrosion caused by temperatures exceeding 700 °C. In the same way, the nickel-based alloy fared better than its iron-based counterpart in both wear and oxidation resistance. The cobalt-based alloy did not exhibit any of the amounts of material removal that the other two alloys did in HTRI tests. The nickel-based alloy had abrasive scratches from tangential sliding but no observable wear that could have been caused by impact. The iron-based alloy displayed wear both from impact and sliding. Based on these results, cobalt-based alloys are better suited to serve under the harsh conditions exhaust valves are subject to than either nickel or iron-based alloys. However, because of the high price of cobalt, it is not always practical to use cobalt alloys for valves. This study suggests that although the nickel-based alloy was not as wear resistant as the cobalt-based alloy, the nickel-based alloy was more effective than the iron-based alloy and seemed suitable for most engines. It is only in the extreme case that a cobalt-based alloy might be needed.

Film Formation of Spin Cast PbSe Quantum Dots

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Chemical treatment typically causes cracking in PbSe quantum dot (QD) films. During attempts to alleviate post chemical treatment film cracking in PbSe QD films, it was discovered that as-made (pre-treatment) spin cast films display surface cracking. The following attempts were made to prevent cracking in as-made spin cast PbSe QD films: 1) Multiple QD batches, made by multiple researchers and with multiple absorption peaks, were used to produce films. 2) Multiple solvents were used to dissolve QDs into solution for film production. 3) Substrate cleaning methods were improved, and multiple substrate

shapes and materials were used. 4) QD solutions were both sonicated and filtered prior to film formation. And 5) Oleic acid was added to dried QDs prior to addition of solvents and before film deposition. None of these methods were able to completely prevent as-made film cracking. However, addition of oleic acid produced optically smooth films that displayed micron scale cracks only under a scanning electron microscope. The success of the oleic acid addition method suggests it may be possible to prevent cracking in as-made PbSe QD spin cast films by perfecting the oleic acid addition method. In order to achieve crack free as-made films, it will be necessary to perform further research on the oleic acid addition method to determine the appropriate volumes of oleic acid required, as well as the ideal time during solution preparation to introduce the additional oleic acid. Once this critical research is completed, the original goal of treating post treatment cracking can be pursued.

Study of the Initial Oxide Scale Formation and Growth on Haynes 214 Alloy

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The initial oxidation process of Haynes 214 alloy was studied to determine the alloy's potential effectiveness in fuel cell stacks and various other high temperature applications. Most often Cr containing alloys are protected by a thin chromium oxide layer on their surface. However, the chromium oxide scales can react with water vapor and oxygen gas in the fuel cell leading to an electrical performance loss by contaminating the fuel cell electrolyte or cathode. In order to prevent this problem, Alumina forming alloys such as Haynes 214 are of great fundamental and technological interest. However, a clear understanding of the actual mechanism of oxide nucleation, growth and precise chemistry are lacking in the existing literature. In order to study the morphology, chemistry and kinetics of the oxide scale, the alloy samples were oxidized in a furnace at 900 °C for different times. The oxide scales were analyzed using various surface and bulk sensitive analysis techniques. The data showed that the oxygen content of the alloy increased rapidly within the first hour of exposure and remained stable up to ten hours. As expected, the surface of the oxides was shown to be alumina rich with minimal chromia formation.

Searching for Anomalous Effect in Gallium Implanted Superconducting Nano-Hetero-Structures

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An anomalous result in superconductivity has been observed in a bi-layer structure consisting of niobium and gold with implanted gallium ions. The objectives of this research are to (a) recreate a bi-layer gold/niobium superconductor thin film structure, (b) utilize the focused ion beam (FIB) technique to implant gallium ions in a selected region within the structure and (c) observe the superconductive transition temperature in another region which is not irradiated directly with a gallium ion beam. The thickness of each layer was approximately 10 nm. The implantation was achieved with a 30 KeV FIB. A nano-scaled bi-layer structure of Nb_{1-x}Ga_x was fabricated with 0 ≤ x ≤ 0.02. The transition temperature from the superconducting phase to the normal-conducting phase is the main parameter evaluated. To isolate the effect, a mask was utilized to form a lateral definition via "lift-off patterning" techniques. The Nb/Au films were deposited on Si-SiO₂ wafers with selected areas removed. In each film, a "window" was created and exposed to the focused Ga⁺ ion beam. Depending on the beam energy and the beam exposure time, the films displayed interesting superconducting properties such as two phase coexistence since the films consist of two regions of superconductive material. By purposely creating two large rectangular pads connected by a narrow bridge, a geometrically defined superconducting film was built. The analysis of preliminary data gathered suggests there may be two transitions as the superconducting transition temperature in the non-implanted sample was lower than that of the implanted superconductor.

Atomic Layer Deposition of Zinc Tin Oxide Thin Films

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Transparent conducting oxides (TCOs) are an essential component of such technologies as flat panel displays, solar cells and solid state lighting. The need for a less expensive, viable TCO has become more urgent due to the widespread demand for TCOs such as indium-tin oxide (ITO) and the expenses associated with producing the most desirable TCOs. One promising TCO is zinc-tin oxide (ZTO). ZTO has been touted as an ITO replacement because both components of ZTO are accessible and inexpensive, and the combination of the two oxides affords increased durability and corrosion resistance to

the material. The atomic layer deposition (ALD) reactor assembled at Argonne National Laboratory is capable of depositing approximately monatomic layers of both zinc and tin oxide using controlled pulses of diethyl zinc and water, and tetrakis (dimethylamino) tin and hydrogen peroxide, respectively. Alternating cycles of ZnO and SnO₂ deposition and changing the relative applications of the two cycles make ZTO deposition possible within very specific parameters. This method grants improved control over composition and thickness (angstrom scale) under reasonable deposition conditions (150–200 °C) when compared to other deposition methods such as magnetron sputtering, filtered vacuum arc deposition and pulsed laser deposition. In this project, thin films of ZTO were deposited using ALD, and the composition and properties of the films were analyzed before and after annealing using ellipsometry, four point probe, X-ray fluorescence, X-ray diffraction (XRD) and scanning electron microscopy measurements. By depositing films of ZTO at 200 °C, resistivities of as low as $2-7 \times 10^{-3}$ were achieved while maintaining transmittances of 80%. While films of ZTO were not as conductive as pure SnO₂ or ITO films, they transmitted light well and XRD analysis revealed that the films possessed an amorphous structure and low surface roughness. Further investigation into the physical properties of ZTO and exploitation of its high transmittance and durability may yield viable applications.

Medical and Health Sciences

Testing the Validity of a Single Administration of the Point Subtraction Aggression Paradigm in Healthy Men

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The Point Subtraction Aggression Paradigm (PSAP) is a performance-based measure of experimentally induced aggression. Several studies have shown that accelerated aggressive responses on the PSAP are associated with higher trait aggression measured by self-report questionnaires. However, the PSAP is commonly applied in multiple administrations in studies testing the efficacy of aggression-reducing pharmacological agents in violent offenders. Little is known of the potential validity of the PSAP in other laboratory situations. This study examined the validity of the PSAP in a single administration in healthy individuals. We hypothesized that the B-choice button press responses on the PSAP would positively correlate with self-reported aggression measures following a single-administration, supporting the concurrent validity of PSAP as an experimentally induced aggression in healthy men with a normal variation on trait aggression. A total of 55 healthy male adult participants, ages ranging from 21 to 46 years and with education from 11 to 20 years, completed the PSAP, performance-based measures and self-report measures of aggression. The results of this study show that the PSAP responses that measure state aggression were uncorrelated with measures of trait aggression obtained through self-reporting measures.

Comparison of Astrocyte Density in the Prefrontal Cortex and Hippocampus of Helpless and Nonhelpless Rats in a Model of Depression

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The prefrontal cortex (PFC) and hippocampus are brain regions implicated in the pathogenesis of depression. The PFC is involved in executive function or decision-making and the hippocampus in learning and memory. These brain areas contain macroglia cells called astrocytes which play an important role in the structural support and maintenance of neurons. Astrocytes have also been found to play an important role in the regulation of neurotransmitters in the extracellular matrix. However, recent research suggests an even more substantial role for astrocytes in terms of mental illness and depression as a change in their number often reflects disease. This event has been shown in several regions of the brain, specifically, the prefrontal cortex and hippocampus where it was discovered that there is a reduction in mRNA expression level for the GABA transporter GAT3 in the hippocampi in a model of depressive-like behavior. Using the same animal model as in the mentioned study, the learned helplessness paradigm via foot shock, we investigated whether this change in mRNA expression corresponded to a change in astrocyte density. Congenital learned helpless (LH) and non-learned helpless (NLH) rats representing depressed and non-depressed conditions, respectively, were selected from a test group of 20 rats to determine their cohort resulting in four rats per group. After the animals were perfused and their brains removed, immunohistochemistry was incorporated to look at the relative densities of astrocytes in the prefrontal cortex and hippocampus. Glial fibrillary acidic protein (GFAP) was used as a marker to indicate

astrocyte presence. GFAP was stained using immunofluorescence with Alexa Fluor. Statistical analysis using a student t-test revealed a significantly higher number of astrocytes in the CA1 region of LH compared to NLH ($p=0.019$). Taken together, these results suggest the increased importance of astrocytes in the pathogenesis of depression. This can lead to improved methods for treatment and better understanding of the cortical-limbic circuitry underlying mental illness.

Effect of Isoflurane on Lactate and Other Metabolites in the Neocortex of Rats Investigated by Proton Magnetic Resonance Spectroscopy (1HMRS)

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Isoflurane (ISO), a popular anesthetic gas, is used on laboratory animals to perform experiments humanely and expediently. However, ISO can lead to concentration-dependent changes in a wide variety of metabolites as shown in previous 1HMRS studies with monkeys. Our experiment tested ISO's influence on concentrations of metabolites in the neocortex of rats compared to that of Nembutal, a general intravenous anesthetic. Using a 9.4 T MRI instrument, 1HMRS scans were performed in the neocortex of each rat. Group 1 rats were exposed to ISO, and Group 2 rats were exposed to Nembutal. Two scans were obtained from each Group 1 rat; one scan was done at 1 minimal alveolar concentration (MAC), and the other was at 2 MAC of ISO. In Group 2 rats, only one scan was performed at 40 mg/kg of Nembutal. All physiological parameters of the rats were kept normal before and during each scan. Conventional software (LC Model) was used to analyze the 1HMRS data. We found that lactate/Cr ratio in Nembutal-anesthetized animals was negligible in comparison to the lactate levels at either MAC of ISO ($p=0.003$ and $p=0.0003$). In addition, there was an increase in the lactate/Cr ratio in the neocortex at 2 MAC compared to 1 MAC of ISO ($p=0.067$, $n=9$). This direct relationship supports the idea that ISO causes an increase in the brain tissue lactate concentration. Importantly, the chemical shifts for lactate and neural stem cells (NSC) are very close to each other (1.33 ppm vs 1.28 ppm) in the 1HMRS, and a high lactate peak in the spectra can blunt the weak NSC signal. Hence, inaccurate data can be obtained if ISO is used as an anesthetic for the animals in NSC research. This comparison suggests NSC researchers should choose Nembutal over ISO to gain better results from their experiments. In future investigations, we will design experiments to understand the mechanisms underlying the ISO-induced lactate increase and its physiological implication.

* Development of Radioligands for Positron Emission Tomography Imaging of Histone Deacetylase and Biodistribution Studies of ¹⁸F-Fluoroacetate

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Deacetylation of histone proteins by histone deacetylase (HDAC) affects transcriptional regulation and contributes to the development of cancer. The development of radiotracers for Positron Emission Tomography (PET) imaging of HDAC may provide tools for understanding the role of these enzymes. We, therefore, attempted to synthesize two ¹¹C-labeled HDAC ligands (a hydroxamic acid and an α -ketoamide) for PET imaging studies. Additionally, we prepared ¹⁸F-fluoroacetate (a possible metabolite of another potential HDAC radiotracer) and studied its in vivo biodistribution. The preparation of the unlabeled target ligands and precursor compounds was undertaken using multi-step synthetic procedures. The target unlabeled hydroxamic acid was successfully prepared in four steps using commercially available reagents, while the synthesis of its corresponding precursor molecule by demethylation of the target compound failed to yield the desired compound. Alternative procedures for the synthesis of the hydroxamic acid precursor are under development. Preparation of the α -ketoamide and its precursor proved to be more challenging and procedures attempted thus far failed to produce key intermediate compounds. Conditions for the synthesis of the ¹¹C-labeled radiotracers together with high performance liquid chromatography (HPLC) conditions for their purification are still to be developed and baboon studies will be attempted in the near future. ¹⁸F-Fluoroacetate has been successfully prepared by heating kryptofix, potassium carbonate, and the corresponding precursor compound in acetonitrile, at 100 °C, for five minutes. Purification conditions were optimized and baboon studies were conducted. Analysis of the PET data suggested very little uptake of ¹⁸F-fluoroacetate in the baboon brain and in most organs but high uptake in the kidneys and bladder, suggesting that the main excretory pathway for this radioligand is via the renal route. The results of these studies may provide valuable information on the distribution and activity of HDACs in diseased

and normal states and therefore allow better understanding of the relationship between genes, brain chemistry, and enzymatic behavior.

Gamma-Vinyl GABA Inhibits Methamphetamine-Induced Reinstatement of Conditioned Place Preference in Rats

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Relapse poses a tremendous challenge to the successful treatment of methamphetamine (METH) addiction. To date, no effective medication exists. Given that the abuse of this potent and highly addictive psychostimulant is growing, investigating possible pharmacological relapse treatments is of the utmost importance. A drug that shows great potential is racemic gamma-vinyl GABA (RS-GVG, Vigabatrin). By irreversibly inhibiting GABA-transaminase, RS-GVG enhances GABAergic transmission and effectively decreases mesolimbic dopamine levels. Past studies have found that RS-GVG inhibits dopamine elevations normally elicited by METH. In addition, it prevents the expression of a CPP to a variety of drugs, suggesting that it can effectively block the incentive motivational value of many drugs of abuse. Moreover, RS-GVG has been shown to inhibit cocaine-triggered reinstatement of rodent reward-seeking behavior, as measured by self-administration. Using the extinction/reinstatement procedure based on the conditioned placed preference (CPP) paradigm as a rodent model of relapse, the present study is the first to investigate the ability of RS-GVG to block METH-induced reinstatement of a METH CPP following a period of extinction in rats. Additionally, four different pairing doses of METH (1.0, 2.5, 5.0, 10.0 mg/kg), administered intraperitoneally (i.p.), were used. After a 20-day conditioning period of alternating 30-min METH and saline pairings, animals in all dosage groups exhibited a strong CPP. With repeated testing in the absence of METH, all preferences were subsequently extinguished (defined as at least six consecutive days with no preference). After extinction, re-exposure to a METH challenge injection produced a consistent reinstatement of the CPP in all dosage groups. Most importantly, this METH-induced reinstatement was inhibited by pretreatment with RS-GVG (300 mg/kg, i.p.) 2.5 hours prior to the METH challenge. The fact that an acute dose of RS-GVG was capable of preventing reinstatement in rats treated with a wide range of METH pairing doses suggests that its potential to effectively prevent METH relapse is broad and robust. Given that re-exposure to the drug itself is a common precipitant of relapse in humans, RS-GVG's potential to block such drug-triggered relapse offers great promise for METH abusers. Future work will focus on examining whether RS-GVG can similarly block reinstatement of a CPP to a variety of other commonly abused drugs.

Protein Crystallography of the Two-Component Copper and Silver Response System, CusR

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The structure of a protein can provide valuable information about its functional mechanisms and its interactions with pharmaceutical drugs. Our research goal was to determine the crystal structure of CusR, a cytoplasmic protein involved in regulating the expression of the proteins that maintain intracellular copper and silver homeostasis. Polymerase chain reaction (PCR) was used to clone the CusR gene from *Escherichia coli* (K12) genomic DNA. This gene was inserted into the vector pET-15b and expressed in the competent cell BL21 (DE3). The expression of the protein was measured with a standard Western Blot technique. Immobilized Metal Affinity Chromatography (IMAC) was used to purify the protein after lysing the cells with a French Press. After purification, the concentration of the protein was measured with an acid, bicinchoninic protein assay (BCA). Using six liters of Luria Broth (LB) medium and an optimized growth period of four hours at room temperature, only about 2–3 mg of protein was obtained, which was concentrated to 20 mg/ml. CusR was then crystallized using hanging drop vapor diffusion with various crystal screening kits. Although some preliminary crystals have been obtained, there is much work left to be done optimizing the crystallization conditions. Also, CusR is apt to precipitate so future work should aim to optimize expression conditions and reduce inclusion body formation.

Binding of Synthetic Growth Factors to Heparin: Optimization of the Release Rate of Fluorescein Labeled Peptides

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Heparin-binding growth factors such as basic fibroblast growth factor (bFGF, a.k.a. FGF-2) and platelet-derived growth factor (PDGF) are important in the wound healing process. Heparin is a glycosaminoglycan that binds growth factors such as bFGF and PDGF. F2A4, a synthetic growth factor developed at BNL that mimics

the natural bFGF, is a multi-domain synthetic peptide consisting of two long chains that bind FGF to receptors, a spacer domain, and finally, a heparin-binding domain (HBD). The ultimate goal of this project was to design a system for loco-regional delivery of this peptide by creating a bioactive surface coating from a heparin plus F2A4 coating that accelerates the healing of wounded tissue. Because of its structure, F2A4, like FGF, binds to heparin. In order to test and modify the heparin-binding properties of F2A4, we used a series of smaller peptides consisting of a fluorescently-tagged HBD sequence in which the number and position of basic amino acid residues act as surrogates for the much larger F2A4 product. From previous experiments, we know the dissociation constant of F2A4 and heparin. This makes it possible to test the kinetics of the release of F2A4 from a heparin-coated surface, and the effect of modifying the sequence of the peptide. The peptides were bound to a black 96-well polystyrene plate coated with silyl-heparin and the fluorescence intensity was measured in a Tecan Ultra Evolution 384 fluorimeter. Alternatively, to determine whether using a different type of heparin would promote a significant difference in the rate of release of the device, we used an avidin-coated plate with biotinylated heparin instead of silyl-heparin. Substituting these materials did not prove significantly more or less effective than using the polystyrene plate. Due to time constraints, final results were not collected for this project, and it will be continued throughout the rest of the summer.

Gamma Vinyl-GABA: A Novel Treatment for the Attenuation of Cue-Induced Drug Relapse

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Addiction lays at the heart of many problems for people and their families. Whether it is to illicit drugs, alcohol, gambling or food, addiction is based on the way the brain processes the neurotransmitter dopamine. After treatment for any addiction, preventing relapse, induced by not only drug administration but various cues as well, poses a significant challenge to the successful management of methamphetamine (METH) dependence. Although no effective medication currently exists for its treatment, racemic gamma vinyl-GABA (R,S-GVG, vigabatrin) shows enormous potential as it blocks both the neurochemical and behavioral effects of a variety of drugs, including METH, heroin, morphine, ethanol, nicotine and cocaine. Using the reinstatement of a conditioned place preference (CPP) as an animal model of relapse, the present study specifically investigated the ability of an acute dose of R,S-GVG to block cue-triggered reinstatement of a METH-induced CPP, utilizing light as the cue. Animals acquired a METH CPP following a 10-day period of conditioning, in which they received five pairings of alternating saline and METH injections. During conditioning, an experimental group was given a dose of 2.5 mg/kg METH (i.p., n=8/group) against a control group. Animals given METH demonstrated a robust and consistent CPP which was then subsequently extinguished with repeated saline administration without light exposure. Upon extinction, the experimental group was expected to reinstate with a cue-induced challenge, but this did not occur. This study showed that light was not effective in serving as a cue that could induce drug relapse.

Treating the 9LGS Rat Brain Tumor with Microbeam Radiation Therapy

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In conventional radiation therapy, the limitation in delivering the adequate dose to the tumor is the damage to the normal surrounding tissue. Microbeam radiation therapy (MRT) is an experimental method that uses arrays of parallel, thin planes of synchrotron-generated X-rays (called microbeams, or microplanar beams). It allows the normal tissue, including the central nervous system (CNS), to recover from these irradiations at doses many times higher than doses from the conventional beams that severely damage the tissue. The effect has been attributed primarily to the quick recovery of the microvasculature due to the survival of angiogenic cells between the microbeams. Additionally, at very high doses, single-direction microbeam irradiation kills the tumor in a single session without damaging the surrounding normal tissues, an effect called "the preferential tumoricidal effect of microbeams". Early MRT studies used very narrow beams, 30–90 μ m thick. However, our recent studies showed that the CNS also tolerates beams as thick as 0.68 mm. We used an array of thick microbeams in a method called "stereotactic microbeam radiation therapy (SMRT)" to treat the rat brain tumor 9L gliosarcoma (9LGS). This method uses irradiations from ten different angles, all crossing the tumor. The crossing of these beams may leave areas of the tumor that are

unaffected. By infusing a solution of iodine and saline into the rats tail vein a dose-smearing affect is achieved. The highly vascular tumor has an increased amount of iodine in the tumor, which could produce localized dose enhancement. The rats were irradiated with SMRT on day 14 after tumor inoculation. Following the irradiation they were weighed and otherwise observed daily. The parameters registered were a) if the rat was lethargic, b) if there is any sign of dry blood around the rat's eyes or nose (which are indications of intracranial pressure produced by the tumor), c) if the rat shows epilation over the head where the radiation was aimed and d) if the rat shows any sign of abnormal behavior (including vocalization upon touch). As of today, 32 days post-inoculation, the results are inconclusive as some rats are losing weight.

Imaging Cue-Induced and Cocaine-Induced Striatal Dopamine Release with 11C-Raclopride PET in Awake, Freely Moving Animals *Courtney Liebling (SMITH COLLEGE, NORTHAMPTON, MA 01063), Wynne Schiffer (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).*

The recent development of positron emission tomography (PET) scanners designed for small laboratory animals has made possible novel neuroimaging studies for a variety of human diseases, including drug addiction. Quantitation in PET studies depends on the measurement of radioactivity concentrations within distinct brain structures. Therefore, a region of interest (ROI) that corresponds to that structure must be defined within the PET image. However, applying the ROI template in the most efficient manner has yet to be determined. This project relies on comparing two different methods using ROI templates to analyze microPET data. In the first method, a region outlining the anatomical borders of the ROI was used. In the second method, a sphere at the center of the anatomical region was used, which accommodates the known limitations of the PET method. These methods were applied to a series of microPET 18FDG scans performed using 20 male Sprague-Dawley rats. After baseline 18FDG scans were performed using an R4 microPET tomograph, rats were alternately administered methamphetamine or saline for four days. Animals then received Gamma-Vinyl-Gaba (GVG) treatment, and following this treatment regimen, animals were again scanned using 18FDG. Forty-five days later, when the animals were adults, they were given an acute challenge of methamphetamine during 18FDG uptake. Increases in brain metabolism were observed in distinct frontal and subcortical regions of the brain with an acute challenge of methamphetamine in rats that were pretreated with only one dose of GVG. These observations were better supported using ROIs that were drawn in the centers of the regions as opposed to ROIs that were drawn around the entire region.

Characterization of Peripheral Glucose Metabolism in Mice with Reduced Expression of the Dopamine Transporter: Differential Modulation by Gender and Insulin Status

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The Dopamine Transporter (DAT) regulates synaptic dopamine (DA) concentrations through its reuptake action of DA. Previous studies have documented decreases in Amphetamine (AMPH) induced DA release and AMPH self-administration in rats rendered hypoinsulinemic after administration of Streptozotocin (STZ), a potent antibiotic that selectively targets and damages insulin-releasing pancreatic beta-cells. Interestingly, insulin replacement therapy reverses the behavioral effects of AMPH in STZ-treated rats. Furthermore, hypoinsulinemic rats show reduced cell surface expression of DAT. Finally, using microPET imaging with 2-[18F]-fluoro-2-deoxy-D-glucose (FDG), mice lacking DAT had significantly higher brain glucose metabolism compared to wild-type mice. These studies suggest that both peripheral and central insulin and glucose metabolism may be involved in the regulation of DA and expression DAT. In this study, we hypothesized that because insulin is shown to diminish DAT expression, mice with reduced DAT expression may differ in glucose metabolism from controls. We investigated peripheral glucose metabolism in male and female DAT wild-type (+/+), heterozygous (+/-) and knockout (-/-) mice before and after peripheral insulin-depletion (220 mg/kg STZ) and subsequent insulin replacement therapy. Peripheral measures of glucose metabolism consisted of plasma concentrations of glucose in response to a 2 g/kg glucose tolerance test (GTT). The most notable finding was in the male DAT +/- whose glucose levels did not peak during the GTT, while DAT +/- mice peaked and then gradually declined. On the other hand, we found that STZ-treated DAT +/- mice showed similar glucose levels compared to wild-type animals. Female DAT +/- mice also showed significantly lower glucose levels compared to control mice and unlike the males, this difference was not reversed by STZ. Mice with reduced expression

of DAT showed significant differences from controls in glucose levels following a GTT and the direction of the difference was dependent upon gender. Insulin-depletion following STZ treatment reversed these differences in male, but not female mice. These findings point to both DAT and gender-related modulation of glucose metabolism. Such findings will aid in advancing our understanding of DAT regulation of metabolism which may contribute to disrupted dopaminergic signaling in disease states such as addiction.

Microbeam Radiation Therapy to Treat the 9LGS Rat Brain Tumor

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Synchrotron sources generate very intense beams of nearly parallel X-rays. These beams can be made into microplanar beams (microbeams) which we use in microbeam radiation therapy (MRT). It has been shown that the normal brain tolerates irradiation with microbeams at much higher doses than conventional beams. Although there is a transient damage to the normal tissues positioned in the direct paths of the microbeams, these tissues seem to recover from this damage better than the cancerous tissues, thus reducing the risk of long-term damage to normal tissue. This recovery is attributed to the fact that the normal capillary blood vessel cells that survive between the microbeams help repair the damage done in the neighboring microvasculature. Therefore, the goal is to use a microbeam radiation method that can saturate the tumor with a complete beam while the segmented beams pass through the tissue with less effect. This is exactly what interlaced microbeams do. This method uses two arrays of microplanar beams aimed at the tumor from 90° angles, which interlace to produce a solid beam at the target. Rats were anesthetized with ketamine/xylazine and injected with 9L gliosarcoma (9LGS) cells in the left side of the brain. The rats were irradiated using the interlaced beam method at day 13 after inoculation and weighed and observed daily following the irradiation. Observations were based on whether or not the rats were sluggish, showed strange behavior (for example, squeaking), had any blood around their eyes or nose, or showed any signs of hair loss. Rats that showed signs of infection were injected with Baytril antibiotic. As of today, eight weeks post-inoculation, 50% of the rats are alive and gaining weight. These results indicate that the interlacing method has a potential for clinical use because of its low impact on the normal tissues surrounding the tumor.

Do Human Mammary Epithelial Cells Synthesizing DNA in S-Phase Have a Greater DNA Damage Marker Response Compared to Other Cell Cycle Phases with X-Rays?

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Breast cancer is the most common cancer among women, resulting in nearly 40000 deaths per year in the United States. While many factors contribute to the development of breast cancer, recent interest has focused on the effects of low-dose radiation on human mammary epithelial cells (HMEC). Many methods for investigation of the potential risk of radiation on HMEC rely on DNA damage-response markers, such as γH2AX, 53BP1 and TP53. In this paper we investigate the response of two HMEC lines to low doses of X-rays (1000–4000 mSv) in order to determine if there is a cell cycle dependence to the DNA damage response markers. We have specifically scored whether there is a difference in DNA damage response markers in S-phase cells compared to non-S-phase cells. Our results indicate that no cell-cycle differences are apparent in cells directly targeted with X-ray exposure and examined promptly after irradiation. Recent published literature indicates that cell cycle differences do exist due to differences in dephosphorylation processing hours after the radiation exposure. For this reason we plan to investigate the kinetics of the DNA damage response markers at longer incubation times after exposure. In addition, we will examine the cell-cycle dependence of "bystander" cells adjacent to neighboring cells targeted with an X-ray microbeam.

Neutral Olfactory Stimulation in a Rat Model of Obesity: Seeking Behavior as Assessed by Nose-Poke Activity and Locomotor Responses in the Open Field

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Food intake is regulated by factors that modulate caloric requirements, as well as food's reinforcing properties. Apart from genetic factors, there are also environmental factors that play a very important role in obesity, including society, culture, stress, food palatability and food availability, as well as food-related cues. Previously, we showed that exposure to an appetitive food stimulus had significant effects on brain glucose in both humans and rodents. Previously, we examined the effect of genetically-induced obesity and food restriction on seeking

and learned behavior before and after classical conditioning of a food (bacon) olfactory stimulus. Zucker Obese (Ob) and Lean (Le) rats were divided into four groups: i) Ob ad lib fed, ii) Ob food restricted (70% of ad-lib), iii) Le ad lib fed and iv) Le food restricted rats. Leptin-receptor deficiency, food restriction, and stimulus conditioning all caused differential responses in locomotor and nose-poke responses to olfactory stimulation. In this study, we replaced the food olfactory stimulus with a novel scent, lavender, and found similar trends. At three months, food-restriction suppressed seeking behavior in both strains; however, at 10 months genetically obese animals exhibited the highest degree of seeking behavior regardless of diet.

* K-Means Clustering to Extract the Arterial Input Function in PET Imaging

Matthew Sabatello (St. Joseph's College, Patchogue, NY 11772), Jean Logan (Brookhaven National Laboratory, Upton, NY 11973). Positron Emission Tomography (PET) is a medical imaging tool used to measure radioactivity in the human body after the injection of a radio-labeled tracer which leads to the creation of a quantitative image that can be used to compare results between subjects. In this study, a K-means clustering algorithm, which was written in C by our research group, was used to extract the input function (radioactivity in the blood) from the early time frames of a PET study. Normally this data is gathered by sampling arterial blood, an often invasive procedure that requires the patient to have an arterial catheter inserted into his or her arm. This algorithm creates groups of Time Activity Curves (TAC) by examining each voxel (3-D pixel) from the PET image and assigning it to a cluster. For example, in our study we used blood, tissue, and background clusters. This procedure is being tested using several tracers to explore the validity of this method, including [11C]methamphetamine and [11C]cocaine. The Imaged Defined Input Function (IDIF), which is the output of the k-means clustering algorithm, is compared to measured arterial plasma radioactivity from the same studies. Before we can use this algorithm, there must be some adjustments made to the image, such as creating a Region of Interest (ROI) around the carotid arteries. The final step was to develop a procedure to estimate the recovery coefficient in order to compensate for the fact that the radioactivity of the carotids in the image underestimates the true radioactivity (partial volume effect). One of the partial volume procedures we developed was to take the ratio of the integral of the IDIF and real blood data curves. Another good procedure applied to these curves was to compute the ratio of their peaks. The results obtained for each tracer were different. For example, the integral partial volume range for [11C]methamphetamine was 0.41–0.63 and the partial volume for [11C]cocaine was 0.22–0.34 and the peak partial volume range was almost identical. The implementation of this algorithm would eliminate the need for test subjects to have a catheter inserted into an artery during a PET scan.

Microbeam Radiation Therapy: Applying the Method to Treat Rats with Stab Wounds in Their Brains

Mark Salomon (University of Michigan, Ann Arbor, MI 48109), Avraham Dilmaman (Brookhaven National Laboratory, Upton, NY 11973). We studied the effects of microbeams on the rat brain subjected to stab wounds. These injuries are very much similar to spinal cord injuries in that they involve the responses of the glial system, an important component of the nervous system, and the immune system. Oligodendrocytes produce myelin and astrocytes hold the blood-brain barrier together and maintain homeostasis in the nervous system. Thus, when the rats' brains are injured the affected tissue relies on the immune system and the glial cells to facilitate healing to the damaged area. This experiment observed the response of the rat glial and immune systems to Microbeam Radiation Therapy (MRT) where neurological damage is present. MRT was used to treat rats with inflicted stab wounds to the brain. The stab-wound rats were irradiated with thin X-ray beams (microbeams) at the National Synchrotron Light Source (NSLS). Rats were injured in their left and right striatum with needle stabs and were irradiated with microbeams of 27 micron thickness. Following irradiation, the rats' weights were tracked over a period of 25 days. Their brains are currently being harvested for immunohistochemistry. The process will be further carried out through the perfusion of the circulatory system and subsequent removal of brain tissues from the deceased stab-wound rats. The aim is to evaluate the immune response and possible presence of demyelination and gliosis. Unfortunately, the stab-wound rats do not display physical characteristics, such as locomotive ability deficiencies seen in a spinal cord injury, which can be used to track their progress post-irradiation. Thus, the stab-wound rats can only be assessed in postmortem histological studies of the brain tissues. These studies are to be carried out by our collaborators at an offsite lab, and the results of these studies

will not be available until September of 2008. Thus, there are currently no results or conclusions.

Forewarning of Epileptic Seizures from Scalp Brain Waves

Ramy Sayed (Middle Tennessee State University, Murfreesboro, TN 37013), Lee Hively (Oak Ridge National Laboratory, Oak Ridge, TN 37831). Epilepsy afflicts about 1% of the world's population. Medication or surgery can help approximately 75% of these individuals, but both of these approaches often have debilitating side effects and/or cognitive impairment. For the 25% of the population suffering from epilepsy, no therapy is yet effective. Seizure forewarning would allow preventive action, reduce morbidity and mortality, and improve epilepsy patients' quality of life. My project involved four tasks. The first was a retrospective analysis of human brain-wave data (electroencephalogram, EEG) to forewarn of epileptic events. This analysis involved 208 datasets, with initial "calibration training" on 60 well-characterized datasets. Calibration training was used to learn to correctly classify cases into pending epileptic events, and non-event cases. Once trained in classifying, the other cases could reliably be categorized with low error rates. The second task was to construct a graphical interface to display the data. In this task, I used the commercial MatLab™ package to display the 19-channel (EEG) data in 30-second windows for each dataset. The interface that I constructed allows a user to mark an event in any of the window(s), scroll forward or backward in time, and change various display features. My third task was to apply the forewarning method to new data in a "blind" analysis, for method validation. The fourth task will be completed later, after the physician has used the classification method to characterize additional cases. The results of my investigations will be included in a manuscript being prepared for a peer-reviewed journal, which I will co-author with Drs. Lee Hively and Nancy Munro. A physician collaborator will monitor EEG data of each patient and will mark the duration of the seizure event of the 141 uncharacterized cases. Dr. Lee Hively's present forewarning methodology will be applied to the same set of complete datasets. We will compare the two sets of observations and will determine the false-positive and false-negative error rates to ensure that the method of seizure forewarning is valid. Our longer-term goal is to develop something akin to the heart defibrillator: when the device recognizes an imminent seizure, certain areas in the brain can be stimulated or certain substances administered to subdue or prevent the impending seizure. The graphical user interface that we created can be used later to construct a seizure-forewarning device for public use.

A Model of Extended-Release Oral Methylphenidate in the Rat

Jessica Steier (State University of New York–Stony Brook, Stony Brook, NY 11790), Gene-Jack Wang (Brookhaven National Laboratory, Upton, NY 11973). Methylphenidate is widely prescribed to children for the treatment of attention deficit hyperactivity disorder (ADHD). Since methylphenidate acts similarly to cocaine, there is concern that the use of methylphenidate in adolescents, particularly in children misdiagnosed with ADHD, might sensitize those children to psychostimulant drugs and leave them vulnerable to the abuse of stimulants later in life. Animal and human studies regarding this issue to date have been equivocal. Most animal studies, however, are plagued by a common problem: the way in which methylphenidate is administered to animals does not resemble the way in which methylphenidate is clinically administered to humans. IP or IV administration of methylphenidate leads to much quicker and higher peak concentrations than seen in the clinical situation in which methylphenidate is taken orally, which is likely to have an effect on the degree to which methylphenidate can sensitize subjects. We have developed an extremely simple method to model the administration of extended release (ER) methylphenidate in rats, which is presented here. Rats were given 8-hour access to methylphenidate solutions mixed to deliver precisely 5, 10 or 15 mg/kg/day as well as dual dosages of 2 and 5 mg/kg/day and 15 and 30 mg/kg/day in which the low dose was administered in the first hour of exposure followed by 7 hours of the high dose; following this exposure, their blood was sampled and assayed for total as well as d- and l-methylphenidate. The dual bottle approach was developed to mimic the clinical extended release administration of Adderall in children. This study shows that restricted 8-hour access to a dual dosage of 15/30 mg/kg solution of methylphenidate achieves serum levels of methylphenidate that closely resemble the outer limits of the pharmacokinetic profile of clinically administered standard doses of ER methylphenidate. The 2/5 mg/kg dual dosage of methylphenidate achieved serum levels of methylphenidate that resemble the lower limits of the clinical standards. This information can be used in the design of further studies to examine the issue of methylphenidate and psychostimulant sensitization.

Optical Detection of Cocaine-Induced Neuronal Function Changes in vivo Using Laser Doppler Flowmetry and Multiwavelength Spectroscopy

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Cocaine use causes cognitive and behavioral changes which can be attributed to its effects on neuronal activity, thus resulting in brain disorders such as addiction and psychosis. The effects of cocaine on neuronal function can be assessed in vivo by optically monitoring cerebral blood flow (CBF), cerebral blood volume (CBV), tissue oxygenation (StO₂) in response to forepaw electrical stimulation before and after acute cocaine administration using Laser Doppler Flowmetry (LDF) and Multiwavelength Spectroscopy (MWS). The rats were anesthetized with isoflurane, intubated, mechanically ventilated and catheterized to monitor and maintain physiological conditions. A craniotomy was then preformed above the right somatosensory cortex centered at 1 mm posterior 4 mm right of the bregma. After surgery anesthesia was switched to α -chloralose to better elicit an electrically-induced response. Then either the LDF or MWS probe was positioned on the surface of the cortex. Electrical stimulations of 2 mA at a frequency of 3 Hz were administered to the left forepaw, and the stimulation-induced changes in CBF, CBV and StO₂ in the somatosensory cortex were recorded before and after cocaine administration (1 mg/kg via a venous catheter). Our results indicate that the forepaw stimulation elicited a ~23% changes in CBF, and concurrent increase of 1–3% in CBV and StO₂ during the baseline. After cocaine, the additional increases of CBF (~5%), CBV and StO₂ (~0.5–1%) were observed in response to the forepaw stimulations. These results validate the functionality of the optical techniques for detecting the hemodynamic at high temporal resolution requires for brain activation studies. Also, the results elucidate cocaine's neurovascular effects to permit a better understanding of the underlying mechanisms by which cocaine acts as a psychostimulant and how its abuse inflicts psychosis.

Learning in High-Functioning Cocaine-Addicted Individuals is Associated with Memory Deficits

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One feature of drug addiction is the persistent use of the drug despite harmful consequences. Such compulsive behavior may be associated with cognitive deficits, particularly in memory and executive function, previously observed in cocaine abusers. Here we (1) compare high-functioning cocaine abusers — substance dependent individuals (SDI) to healthy control subjects (NML) on performance on a classical neuropsychological executive function task, the Wisconsin Card Sorting Task (WCST); (2) use all WCST repetitions to perform an in-depth examination of the group differences in learning; and (3) evaluate how selected cognitive and motivational factors may contribute to perseverative errors on this task. Sixty-two NML and 62 gender-, age- and education-matched SDI completed a computerized version of the WCST. The sample was divided into two groups: those who could not complete all WCST repetitions (SDI, n=29; NML, n=16) vs. those who could (SDI, n=33; NML, n=46). To decrease the impact on results of factors associated with low education and socio-economic status, the non-completers were excluded from further analyses. Participants also completed a learning and memory test, the California Verbal Learning Test (CVLT), and a state measure of self-reported motivation. Results showed that there were no differences in perseverative errors between the high-functioning SDI and NML groups. However, NML showed decreased number of perseverative errors as a function of repetition ($F=4.9$, $p>0.05$), while SDI did not ($F=4.9$, $p>0.05$). Further, memory capacity (learning curve on the CVLT) predicted perseverative errors in SDI.

Analysis of the Biological Effects of Aspirated Carbon Nanohorn Particles in Mice Using Scanning Near-Field Ultrasound Holography

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Engineered nanomaterials, because of their enhanced physicochemical properties compared to their bulk form, are finding an increasingly important role in many potential commercial applications. However, the health effects of nanomaterials are not well understood or thoroughly investigated. Therefore, more studies are needed to examine different types of nanomaterials and the biological responses they invoke. The purpose of this research was to examine the effects of aspirating single-walled carbon nanohorns (SWCNHs) in vivo using mice. Bronchoalveolar lavage (BAL) and blood samples were collected from

two experimental groups, the exposed nanohorn and the control mice. Three mice from both groups were sacrificed 24 hours and seven days after aspiration. Gross examination of the number of macrophages versus activated macrophages in BAL samples from the exposed and the control mice suggested a possible pro-inflammatory response to the carbon nanohorns. Employing a unique detection technique, scanning near-field ultrasound holography, carbon nanohorns were discovered bound to cell membranes, inside cells, and near cells in both the red blood cells (RBCs) and BAL sample cells. The positioning of carbon nanohorns inside the cells not bound to a membrane suggests that they entered the cell through a process other than phagocytosis. Furthermore, the RBCs in all the exposed blood samples exhibited a distorted phenotype. Such distortions could possibly lead to various pulmonary diseases. From their ability to permeate membranes, cause pro-inflammatory responses, and distort the phenotype of RBCs, it can be concluded that carbon nanohorns may pose a biological threat.

* Microbeam Radiation Therapy: Studying the Effects on the Rat Spinal Cord

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Studies of microbeam radiation therapy have shown that the use of thin parallel synchrotron generated X-rays (microbeams) can not only spare normal tissues, but have also been known to help in the process of remyelination and regeneration of glial cells that have been damaged in the central nervous system. As an extension of recent spinal cord injury studies done at Brookhaven National Lab, 14 Long Evans rats were subjected to a spinal cord injury and irradiated several days afterward, using much smaller doses than those of earlier experiments. For control purposes, another group of Long Evans rats were afflicted with the same injury, but were not irradiated. The region of interest for this experiment was between the T9 and T10 vertebrae in which a laminectomy was performed to expose the spinal cord. The contusion was then delivered by the NYU impactor to ensure paralysis from the area of interest and downward. After surgery, the rats were monitored and placed on heating pads to maintain homeostasis. Several days later, the experimental group was irradiated at the National Synchrotron Light Source on the X17B1 beam line. Approximately a week later, the rats were then field-tested using the Basso, Beattie, Bresnahan Locomotor Rating Scale to check for improvements in their walking capabilities. Although the rats are all improving in their performances, the results are not yet conclusive because the experiment ran past the estimated summer term and will be finished at a later date. Future spinal cord research is scheduled to help further the understanding of this biological phenomenon.

Designing a Reward Devaluation fMRI Task

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Drug-associated stimuli can be effectively used to study compromised functions, such as emotional learning and flexible behavioral control, in drug addicted individuals. In particular, monetary reward and salient picture cues are of interest in examining the role of selected prefrontal brain regions in the ability of drug-addicted individuals to acquire, retain, and forgo drug-cue associations. The goal of the current project was to design a classical conditioning task that uses arousing images and monetary reward as the unconditioned stimuli (US) for functional neuroimaging studies. Specifically, our current reward design was adopted from classical conditioning models that utilize potent fear-evoking stimuli as the US. This design consists of two tasks comprised of three distinct phases. During the acquisition phase (Phase I, Day 1), one neutral stimulus serves as the first (most salient) conditioned stimulus target (CS+STgt), and another neutral stimulus serves as the second (less salient) conditioned stimulus (CS+nSTgt); both stimuli are paired with the US (\$4 and \$1 monetary reward, respectively). A third neutral conditioned stimulus (CS-) is never paired with the US (\$0: non-reward); the reward or non-reward pairing is maintained in 70% of the trials. During Extinction Learning (Phase II, Day 1) and Extinction Retention (Phase III, Day 2) phases, all of the CS+ stimuli are unpaired from the monetary reward (US). In the picture-viewing task, monetary reward is replaced by pleasant, neutral, and cocaine images. For both tasks, the US is withheld in the latter two phases to ensure that the conditioned response is diminished or disappears entirely. During task performance, physiological measurements will include functional magnetic resonance imaging (fMRI) blood oxygen level dependence responses in selected brain regions and the skin conductance response which measures autonomic arousal levels. Similarly, subjective ratings, a forced-choice task and post-task questionnaires will serve as behavioral measures in evaluating success of conditioning

and extinction manipulations. These experimental measures and hypothesis validation will be completed after subject recruitment in the subsequent stages of the paradigm. Once implemented, we expect to examine impairments in the brain regions associated with reward conditioning and devaluation in drug addicted individuals, which may prove prognostic for drug craving and compulsive drug use.

Nuclear Science

Analyzing the Failure of Photomultiplier Tubes Under Hydrostatic Pressure

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For neutrino detection experiments such as the Homestake 300Kt project, it is often necessary to suspend spherical arrays of photomultiplier tubes (PMTs) in scintillating liquids such as water or liquid argon. The implosion of these PMTs under hydrostatic pressure presents the need for a better understanding of their behavior when submerged so that costly accidents can be prevented. A statistical model for the structural failure of Hamamatsu R7081/NG PMTs is being developed which seeks to determine the factors controlling a particular tube's peak survivable hydrostatic pressure, including the correlation between pressure shockwaves at the time of implosion and the potential for mechanical initiation of implosion of adjacent PMTs. Research began with the creation of an experimental database of PMT pressure tests and cycles since March 2007, followed by a secondary database analyzing the variations in glass thickness in each of the tested tubes. The analysis showed that thickness in various regions of the PMT glass had a negligible effect on maximum hydrostatic pressure, as did structural defects such as glass flaws. The pressure pulse data generated by each tube's failure were first matched against corresponding CCD camera data. This showed us that the vast majority of the pulse information was corrupted by reflection within the pressure vessel, meaning that only the initial pulse could be used for analysis. Data from each initial pulse was then fit to a normal distribution to determine what factors were common among all of the PMTs. Analysis of each pulse's rise time and shape showed that in all of the R7081 tests, the plastic base of the tube breached the crown immediately after implosion. Consequently, the structure of the PMT glass itself has very little to do with the implosion of the tube, and the integrity of the base varies by 200% in some of our results. Future studies might attempt to create a model based on an alternative distribution, use pre-written fluid dynamics simulation software, or simply create similar models for other PMTs. Our model for R7081/NG failure is expected to provide a reasonably accurate reflection of PMT implosion, and could be used as an alternative to physical testing.

Feedback Control System for Laser Power Recycling Cavity Stabilization

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At the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, a technology based on laser-ion interaction, i.e., laser stripping, was developed to strip off electrons from the accelerated hydrogen ion beam and, therefore, to provide high energy protons. The laser stripping technology can eliminate a number of issues associated with the conventional carbon foil stripping scheme which includes radioactive waste, foil lifetime, and uncontrolled losses due to multiple transversals of the stripping foil by stored protons. Recently, a 90% efficiency laser stripping was obtained over a time period of about 7 ns at a repetition rate of 30 Hz by using a Q-switched solid-state laser. In order to achieve the full-cycle laser stripping, the laser pulses need to match the temporal structure of the hydrogen ion beam at the SNS linear accelerator, which in turn requires a pico-second pulsed laser system with an unrealistic average power (~10 KW). In order to produce high repetition rate, high peak power laser pulses required for laser stripping, a laser power recycling cavity was proposed in conjunction with a frequency tripled macropulse solid-state laser system. This study focused on the implementation of a feedback control system for the stabilization of the optical cavity using a Field Programmable Gate Array (FPGA) to process the error signal generated by polarization dependent optical elements. The proof-of-principle experimental setup used a semiconductor laser, a polarization beam splitter, and a half-wave plate (HWP) mounted on a rotational stage to simulate the feedback loop of the recycling cavity. A program on the FPGA (created with LabVIEW) differentiated the signals from two photo detectors corresponding to two polarization directions to generate the simulated cavity error signal. The simulated error signal was processed to calculate the corrections needed in the cavity and made the appropriate adjustment to the angle of the HWP, thereby completing the

control loop. The feedback system was implemented and a successful experimental demonstration was achieved. Furthermore, the feedback signal was applied to a Fabry-Perot resonator via piezoelectric spacers to study the dynamic response. The results showed the entire feedback system had a bandwidth of up to 5 KHz. The completed program will control the stabilization of the laser power recycling cavity which will be utilized to perform the full-cycle laser stripping.

Analysis of International Thermonuclear Experimental Reactor's Draining and Drying Operations

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With the increasing demand for alternative energy sources, the International Thermonuclear Experimental Reactor (ITER) plans to use fusion as an energy source in attempts to design and operate the first electricity-generating fusion power plant. ITER is designed to explore and test plasma behavior during the fusion burning plasma regime. The data and design will provide plasma control tools to help ITER move toward using fusion as an energy source. The focus of this study was to verify the draining and drying systems of an existing design of a fusion reactor water cooling system. Through the use of modeling and simulation we were able to find parameters for the draining and drying operations. The simulation platform used was FlowJava and the models were written in Python, an object oriented computer language adapted as a scripting medium for FlowJava. Two types of Counter Current Flow Limitation (CCFL) criteria correlations were used in modeling the draining operation. The CCFL criteria allow using the hydraulic diameter of the fluid channel to obtain the gas velocity to drain the water channels. The Wallis-type correlation indicated larger velocities as the hydraulic diameter increased. The Kutateladze-type correlation stayed constant at 2.85 m/s as the hydraulic diameter increased. In the drying operation input values were manipulated to find energy balancing equation conditions. We were able to find the amount of heat required in kilowatts for the drying operation. This research verified that the given parameters of an existing design were similar to the parameters found through modeling and simulation of ITER's design. Some calculations were off by a slight rounding precision, while others were off because of an unknown value that was used in the existing design and not ITER's design. However, we believe the parameters that were found for the draining and drying operations are accurate for the ITER design. Furthermore, research will continue to investigate the parameters of the draining and drying operations along with the ITER water cooling system in its entirety. As a future teacher, the value of this research shows the importance of finding new energy sources and ways to implement research and analysis in the classroom.

An Analysis of Post-Irradiation Damage on CdZnTe Crystal Detectors

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CdZnTe (CZT), a crystal alloy of cadmium telluride and zinc telluride, is currently being researched as one of the leading materials to be used in gamma and neutron detectors. Unlike rival materials such as germanium, which require liquid nitrogen cooling, CZT possesses the phenomenal ability to operate at room temperature. These crystals are currently being researched for suitable applications in detector technology, primarily for implementation in space exploration satellites and utilization in portable-field isotopic identification instruments for homeland security operations. To fully utilize them for these purposes, however, their behavior in conditions likely to be encountered in the field must be fully characterized and understood. At Brookhaven National Laboratory, we are currently studying one of these conditions, the damage degradation of CZT crystals when exposed to massive doses of radiation. Two spectroscopy grade CZT crystals used for detection device technology were irradiated with dosages of 200 MeV protons to simulate harsh radiation conditions in order to observe the physical/chemical alterations in crystal detector properties. Gamma-ray spectra of the crystal detectors were monitored using a high-purity germanium ORTEC detector. Resistance Analyses and Leakage Current were also undertaken to denote changes in the crystals' electrical properties; and since CZT is transparent to infrared light, inclusions and physical damage were observed using an infrared light source. After fluences of $+5 \times 10^9$ p/cm² are induced upon these crystals, dramatic detector performance degradation can be observed. In other works, degradation in the crystal's detection properties are attributed to electron trapping in the crystals. Through this research, we were able to identify the radioactive isotopes activated within the crystal structure after withstanding these extreme radiation conditions. Based on these results, scientists may want to revisit the idea of using CZT crystals for

detection technology; once these radioactive isotopes are activated, it will be impossible to determine whether readings from a damaged CZT detector are from a potentially dangerous radioactive source or the CZT crystal itself. Repair processes by means of heating and annealing will be researched in the near future.

Designing and Constructing a Fabry-Pérot Cavity for the Hall C Compton Polarimeter

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Hall C of Jefferson Lab uses a Møller Polarimeter to measure the polarization of the electron beam, and is going to supplement it with a Compton Polarimeter to provide an independent, non-destructive polarization measurement. Existing designs for Compton Polarimeters generally rely on continuous wave lasers. Hall C will use a green, RF-pulsed, high-power laser, possibly paired with a Fabry-Pérot optical cavity (with a minimum amplification gain of ten). These components will maximize the luminosity of the system which allows for a quicker polarization measurement to be performed. The focus of this project was to clarify whether a non mode-locked pulsed laser system can be used in conjunction with a Fabry-Pérot cavity to produce a large cavity gain. First, the optimal geometry for the Fabry-Pérot cavity was determined in combination with the constraints imposed by the laser and electron beams. From these calculations, a rough "test cavity" was constructed from readily available materials to investigate the compatibility of a non mode-locked pulsed laser system with a Fabry-Pérot cavity. It was found that the best luminosity for the pulsed laser is achieved for a cavity of length 120 cm, with a transverse electron beam size of 50 μm , and a laser beam size of 30 μm . Preliminary results suggest that a Fabry-Pérot cavity will not be feasible in this situation. Longer cavities reduce the time needed for a measurement due to the smaller crossing angle; however, the space for the polarimeter is limited, placing an upper limit on the length of the cavity. It should also be noted that the results for the optimum beam sizes are optimistic, with a more realistic size on the order of 100 μm . The Fabry-Pérot cavity was ineffective because the light produced from the primary laser was not coherent from pulse-to-pulse. However, it may be possible to create this coherence using additional feedback techniques. These findings will now allow Hall C to complete the design of the Compton Polarimeter, which will make polarization measurements in the least amount of time possible, causing minimal disturbances to ongoing experiments. This pulsed laser system may also be integrated into other experimental facilities as needed for this same purpose.

Nuclear Material Control and Accountability: The Efforts Made and the Lessons Learned

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An effort is being made to reduce the inventory of nuclear material at Argonne National Laboratory. One facility of importance is the Alpha Gamma Hot Cell Facility (AGHCF). Before such an effort can be undertaken, the engineers and technicians in the Nuclear Operations Division (NOD) must have an accurate and informative inventory database. The Fissile Inventory Management System (FIMS) was built with several components and is relied upon for logistics, material control and accountability, criticality safety, and the continuity of decades of programmatic data. Because of the size of the database and the operational importance and requirements within the NOD, FIMS is scrutinized and checked to verify the data accuracy. Two major components (tables) in FIMS are the Fissile Ledger Table and the File Card Table. Some components (tables) of data do not overlap from one component (table) to the other. While both tables give data for the amount of fissile material (Uranium-233, Uranium-235, and Plutonium-239), only the Fissile Ledger provides data for other Department of Energy (DOE) accountable nuclear materials. For example: A piece of material may appear to be insignificant according to the data in the File Card Table, but may actually contain Lithium-6 (or other accountable material) according to the Fissile Ledger. The reconciliation of FIMS database tables can reestablish confidence in the accuracy of the NOD inventory and the control of its facilities. In order for the NOD to complete its work to remove material from the AGHCF, the FIMS database must be appropriately maintained to the level of confidence required to do the necessary work. At present, 140 discrepancies have been resolved and may be rebooked with 373 items still requiring attention. Additional effort is needed to reconcile the remaining items. While it is important to correct the information differences between the FIMS Fissile Ledger and the File Card Tables, additional actions must be taken in the future to correct other information in the system. For example: more detailed locations of fuel segments are needed

in the near future in order to increase the efficiency of outgoing fuel shipments. Nevertheless, the corrections undertaken thus far represent a step forward in establishing a more reliable inventory system for the NOD at Argonne National Laboratory.

Design Improvements for the Global Nuclear Energy Partnership Voloxidizer

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Oak Ridge National Laboratory is demonstrating methods for advanced processing of spent nuclear fuel as part of the Global Nuclear Energy Partnership. One of these advanced processes involves the operation of a specialized tube furnace called a voloxidizer. The voloxidizer achieves four reprocessing functions: oxidizing spent nuclear fuel powder to facilitate reprocessing; volatilizing fission gases captured in the fuel separating spent nuclear fuel from its metal cladding; and packaging fuel powder for transport. My internship concentrated on performing one cold-test (no fuel) on the voloxidizer and redesigning several of the mechanical subcomponents to improve its overall performance. A cold-test of the voloxidizer was conducted to confirm the operation of mechanical rotating parts and the electric heaters. After setting up the voloxidizer and instrumenting with thermocouples, we monitored the voloxidizer's performance as the heaters brought the temperature up to approximately 600 °C over a seven-hour period. I recorded data on the temperature increase and observed the fuel basket rotate internal to the voloxidizer. The results of the test showed that the components achieved the expected temperatures; however, we determined that the air distribution tube inside the basket probably should be relocated. I used Solid Works, a 3-D modeling program, to redesign the air distribution system, the product container, and other miscellaneous parts. The air distribution tube will be relocated to the side of the basket, to provide more space for the fuel to tumble. Changing the position of the air distribution tube also required redesigning where the tube penetrated through the drum flange. A new lifting apparatus is needed to accommodate the changes to the air supply tube as well as lift the basket out of the drum, using remote manipulators and an over head crane. I am currently designing a remote lifting mechanism to extract the basket from the voloxidizer drum when the voloxidizer is used in a hot-cell. The new components that I have designed for the voloxidizer are being ordered; when they arrive, the voloxidizer will be retested. Following additional cold-tests, the equipment will be installed in a radioactive hot-cell facility, where the unit can be tested with spent nuclear reactor fuel.

Absolute HPGc Detector Calibration and Evaluation of ^{40}K Radioactive Decay

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Carbon dating is a reliable method for dating old objects that were once alive up to 60000 years ago. A method called Potassium-Argon (K-Ar) dating is used to measure the age of rocks, most of which were created millions of years ago. This is accomplished by measuring the ratio of ^{40}K to the inert gas ^{40}Ar using the assumption that no ^{40}Ar was retained in any qualitative amount during the formation of the rock due to thermal evaporation and the branching ratio of the potassium isotope into stable argon. Being the only viable technique for the dating of very old archeological materials, a more accurate measurement of the half-life of ^{40}K is needed. Using a High Purity Germanium (HPGe) detector and 5 absolute sources, the detector was calibrated and a cylindrical sample of KCl was placed parallel to the detector axis to measure the decay rate of ^{40}K . Using ^{137}Cs , ^{22}Na , ^{60}Co , ^{133}Ba and ^{241}Am with known activity levels, the HPGe detector was calibrated from 2, 4, 6 and 8 inches. Following the calibration, a 2" cylindrical sample of KCl was placed at varying distances from the detector as well as ^{60}Co behind the KCl sample at these same distances in order to calculate the attenuation coefficient in the KCl for the 1460 keV gamma-ray of ^{40}K . The results generated from the data produced a difference of a factor of 2 in the half-life measurement of ^{40}K when compared to previous evaluations of the potassium isotope. The resulting 500 million year measurement compared to the current most accepted half-life evaluation of 1.277 billion years is unknown, as rigorous precautions were taken in every step of the experiment. However, speculations as to the accuracy of the Simpson's numerical integration method used to determine the variation in gamma-ray detection due to attenuation are considered.

Developing Software for Nuclear Process Monitoring by a System of Load Cells

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Nuclear material diversion events are more likely to occur at uranium enrichment facilities in material feed and withdrawal areas. The ability to effectively monitor these processes should significantly enhance nuclear safeguards by providing timely detection of process anomalies that may represent attempts to divert material. A system of continuous load cell monitoring was designed and developed to begin to evaluate the effectiveness of continuous feed and withdrawal monitoring. Software was designed to create a database structure, a user interface, and data acquisition. Specifically, the design and production of this software involved interfacing with a series of load cells set up to model a generic feed and withdrawal process and create a user friendly database solution that supports authentication. This model demonstrates the feasibility to dynamically monitor (F&W) process for safeguards purposes. The system consists of eight load cells connected by a simple serial cable to transfer data from the load cell reader to a communications hub, where the serial cables are interpreted as standard communication (COM) ports. Standard object oriented programming techniques were used to create a hierarchical class structure for the user interface, which was written in the C# programming language. The program is event driven and uses a periodic timer to create events, given the necessarily cyclic nature of retrieving data from the scales. Retrieved, data is stored in a database written in the PostgreSQL language. The software interfaces with the current system of load cells appropriately and has successfully been used in several demonstrations of the system. Overall, this project is valuable because it both meets its requirements by providing a working user interface with the load cells and provides a framework for future projects by being modular enough to allow for great variation in the type of monitored devices used.

Improving the Reliability Model of a Digital Feedwater Control System

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A Digital Feedwater Control System (DFWCS) is a system that controls feedwater to a reactor. The defining feature of a DFWCS is that it operates in digital as opposed to analogue mode. To gain a better understanding of all DFWCSs, one particular DFWCS was analyzed in this study. This particular DFWCS exists in the secondary loop of a pressurized water reactor (PWR). Software was developed at Brookhaven National Laboratory to simulate a DFWCS in order to determine whether a component failure or combination of component failures would cause the entire system to fail. A system failure is defined to occur when the DFWCS switches from automatic to manual mode. For the DFWCS under consideration, possible causes for this switch are quantified in a DFWCS simulator program (which was developed at Brookhaven National Laboratory). My role in this project was to amend the simulator program code to better model the DFWCS under consideration. A quantification program (developed at Brookhaven National Laboratory) is able to calculate and attach probabilities of failure to each component in the system. This data can be fed to a specific kind of mathematical model known as a Markov Model that can be used to determine system reliability. At present, a strong DFWCS simulator program exists, but there is still room for improvement with regard to the programmed modes of failure. The following tasks were undertaken for this project: existing data was taken from Feedwater Control System (FCS) Simulation Software; the data was run through a Markov Model; it was verified that it was possible to produce system failure probabilities comparable to those predicted by previous runs. Next, the software was improved by the modification of the software code to include component/s failures that were not included in the original code. Furthermore, combined failure modes were broken into constituting failure modes such that the model more explicitly accounts for individual failure modes. The improved software was used to simulate the FCS to acquire data about all of the component/s failures that led to system failure. In the future, this data will be fed into a Markov Model in order to determine the reliability of the DFWCS. This work will enable the determination of a more accurate result for the probability of system failure than was previously obtained.

Implementation of Procedures and Surveillance Requirements in the Nuclear Operations Division

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The purpose of this project is to create, reformat, and make additions to procedures and surveillance requirements that are to be implemented into various procedure manuals for the Nuclear Operations Division. The procedures are necessary for the successful operation of many different tasks around Argonne National Laboratory (Argonne). The surveillance requirements are necessary to keep equipment safe and functional through routine check-ups, calibrations, and repairs, if necessary. The majority of these new documents are created from the use of existing procedures and surveillance requirement documents, as well as other manuals such as the Environment Safety and Health manual. The sources can be found online, on a shared Argonne Server, or in hard copy form. These documents must also be reformatted so that there is a universal style represented in each manual. Additions must be made if there is an insufficient amount of information for a specific topic or if a section is missing within the procedure. The procedures and surveillance requirements are governed by DOE orders and must go through several revisions before they are finalized and printed into their respective manuals.

Simulation of High Power Electromagnetic Wave Heating in a Fusion Plasma

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Fusion is the process of fusing two elements, typically deuterium and tritium, to produce energy. This energy or heating of plasma is what we are trying to understand. The use of radio frequency (RF) power using tens of MW of power at 50–100 MHz is one way to reach the 100 million degree temperatures needed to produce useful power. One of the possible effects of RF heating is the formation of a tail in the plasma distribution function. Tails are high energy, non-thermal particles that are the product of the RF heating. In order to study these effects, we are using the all order spectral algorithm (AORSA) and quasi linear 3-D (CQL3D) programs. These programs are used to model how the tails should evolve in time. The results for each point in time are in separate computer files, which are generated from AORSA and CQL3D. Before, programming diagnostic tools for visualization of time-dependent data, has been a manual process. The processing by AORSA and CQL3D makes simulated data to compare with experimental data from Alcator C-Mod experiments at MIT for the present effort. The diagnostic tools which are computer programs to do visualization of time-dependent data are encoded in Python, and the graphical output uses the Python interface to Gnuplot (a 3-D graphics engine) as well as a Python module to read the Network Common Data Form (NETCDF) files that contain the CQL3D output. All are public domain programs that can be used on any computer platform. The diagnostic tools made during this research will bring us closer to being able to understand how the tails are created and what controls their evolution in time.

Comparison of Commercially Available Handheld Radiation Detector/Spectrometers

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Five different handheld radiation detector/spectrometers were tested to determine and evaluate differences in their internal structure, their performance, and other aspects that will affect their potential practical use in the field. The devices used were the IdentIFINDER produced by icx™, Interceptor produced by Thermo and icx™, the GR-135 produced by SAIC®, the GR-135 PLUS produced by SAIC® and the Ortec® Detective-EX-100 produced by Ametek®. Each detector was tested in the same location simultaneously, for various different locations and levels of shielding, including small unshielded naturally-occurring sources (such as Thorium), and large sources through heavily-shielded buildings being used throughout Brookhaven Laboratory. Each detector has its own strong point. The display and organization of the IdentIFINDER appear easy-to-use, with minimal instruction required, and this unit has a high capability for neutron radiation detection. The GR-135 appears to work very well for gamma radiation spectrometry, and the GR-135 PLUS has a larger radionuclide library, as well as the ability to detect neutron radiation. The Interceptor is compact and discreet, while the Detective has the highest resolution of the units tested during this study. As each detector/spectrometer has a strong point, they each have weak points as well. These together dictate whether or not a detector is able to be used practically in the field by radiological response or law enforcement teams. Intuitive layout and controls, and quality of resolution are the two most important specifications, implying that a combination of detectors to be used together in the field would be optimal.

Developing Genomics-Scale Throughput for Small Angle X-Ray Scattering at the Advanced Light Source

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Scattering experiments over the past century are at the base of our knowledge and understanding of matter. The early Rutherford measurements have taught us that the atom has a compact nucleus consisting of nucleons, protons and neutrons, surrounded by orbiting electrons. Subsequent scattering experiments, first performed at the SLAC National Accelerator Laboratory in the 1960's, have revealed that the nucleons themselves have a complex substructure consisting of quarks and anti-quarks that are bound by gluons. Presently, it is known that gluons make up very large parts of nuclear matter and yet very little is known concerning the gluon momentum distribution in the nucleus. The binding, confinement, is a frontier question in nuclear physics. In this work, estimates are made for the kinematic coverage and statistical precision for a scattering experiment of highly energetic electron and nuclear beams at a proposed future electron-ion collider. It is shown that the nucleon can be probed at unprecedented small distance scales with collisions of electron beams of 10 GeV energy and 100 GeV nuclear beams. Such measurements will probe gluons inside the nucleon for a very wide range in momenta, extending to five times smaller values than could be probed so far. Projections of the statistical precision of such measurements are made and show that the future electron-ion collider data will distinguish between current theoretical expectations. The measurements thus give new insights in the unsolved problem of nuclear confinement and the theory of quark and gluon interaction.

Design of an Experiment to Examine Molten Salt as a Heat Transfer Medium

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This study supports the Advanced High Temperature Reactor (AHTR) concept, a high temperature molten salt cooled reactor design, by designing a simplified experiment to study the corrosion characteristics of molten salts. Historically, corrosion studies have been performed using relatively complicated natural circulation loops. The objective here is to determine if a simplified natural convection geometry can be used to acquire data on the corrosivity of molten salt (LiF-NaF-KF). The test unit is 76 cm tall and uses a furnace to heat a pool of molten salt in a nickel crucible. A heated nickel rod is submerged in the center of the molten salt to initiate the natural convection circulation. Using the proposed geometry, the experiment can be implemented at a lower cost and smaller scale compared to natural circulation loops. We completed a thermal analysis before the experiment was performed. Known parameters are entered into the computer algebra system, Mathematica, to perform the calculations. The calculations are plotted in Excel to obtain values for temperature, salt velocity, heat flux and heat loss. The computational fluid dynamics software, FLUENT, numerically simulates flow patterns in the molten salt that result from natural convection. During the experiment, salt velocity is measured by Laser Doppler Velocimetry using a Class IV 514.5-nm laser probe and 899-mm convex lens. Temperature values are measured using thermocouples. An infrared camera will capture pictures of the salt through sapphire viewports. The Excel plots revealed a maximum velocity of approximately 4 cm/s, depending on the radial distance and height from the bottom of the central heater. These plots are based on a temperature range of 700 and 740 °C between the heater and the bulk of the molten salt. FLUENT flow patterns show the natural convection movement that is needed to accurately simulate corrosion characteristics on the nickel surfaces that exist in real reactors. Experiments are scheduled for August 2008. We will compare the empirical results of these experiments to the numerical results to test the model's validity. The analysis of the natural convection geometry provides valuable information to demonstrate that the smaller design can be used to acquire data in the same way as full-sized authentic circulation loops. Multiple, simplified, natural convection experiments can be conducted to test heater rods of different materials and sizes.

Characterization of the Institut Laue-Langevin (ILL) Cryofurnace and Integration into the Sample Environment Suite for Neutron Scattering Experiments

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Controlled sample environments for neutron-scattering experiments are frequently required to provide an extensive range of temperatures from

1.5 to 600K. Commercially available Cryofurnaces advertise a suitable temperature range, yet the methods for operating Cryofurnaces have not been optimized. The goals of this research are captured in two main ideas. First is to define the key operational parameters for the Cryofurnace, such as stable operating temperatures, range of operating temperatures, and cryogen economies. The second is to adapt the equipment to fully support the sample environment. Using information from previous experiments and current temperature dependent studies, I developed a standard step-scan program for testing the Cryofurnace. I conducted low- and high-temperature scans while recording temperature stability, cryogen economy, and temperature range, over changes in time. I collected data using a Labview interface with a Lakeshore model 340 temperature controller; these allowed me to determine the optimum mode of operation. The characterization revealed several unique configurations. An external power supply was added to the system to extend the temperature range. The controller was tuned to obtain a stable maximum temperature, while still allowing the unit to cool at sustainable rates to base temperature. Liquid nitrogen and liquid helium were interchanged within inner chambers to increase economy of operation. I discovered that an "auto-fill" feature for the liquid nitrogen should be used, due to its rapid consumption within the Cryofurnace. I used all of these revealed capabilities to optimize the performance of the Cryofurnace, which allowed the sample environment to be operated in an efficient and user-friendly manner. Further, this research enables the neutron scattering community access to a sample environment that meets the needs of various experiments.

Integrating the Infield Search System with the RadTrac Source Tracking System

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RadTrac is a system used to detect the presence of radioactive sources, determine their position, and track their movement in real time. It relies on external radiation sensors to provide the information it needs to track a source. Previously, RadTrac only supported data collection from sodium iodide detectors connected to the Ortec Digibase photomultiplier tube base with integrated voltage, preamplifier and digital multi-channel analyzer. RadTrac now supports data collection from both the Ortec Digibase and the Infield search system. The Infield systems are connected to Silex SX-500 serial servers which are connected to a generic network switch. A Windows PC running RadTrac is connected to the network switch. The Silex serial servers operate on a TCP/IP based network. Software supplied with the Silex serial servers allows them to emulate a COM port on the computer on which RadTrac is running. RadTrac uses a multi-threaded computing model to collect data from the Infield systems. When RadTrac is instructed to collect data, it searches all active COM ports for active detectors. For each detector that it finds it starts a separate thread which is responsible for handling that detector. This contrasts with the typical computer program that uses only one thread or path of execution. All programming instructions are executed in a sequential manner by the computer. In a multi-threaded program, programming instructions are executed sequentially on each thread with multiple threads executing in parallel. When multiple processor cores are present (as in modern processors) the operating system automatically distributes threads to lesser-used cores which speeds up the overall execution time. In addition, with parallel thread execution the program does not have to wait for data to be retrieved from external devices. One benefit is that the graphical user interface can be updated more often resulting in less image lag. Each thread that RadTrac starts is responsible for collecting data from one detector. The threads use a messaging system to communicate with a supervisory thread. To retrieve data from a detector, the main thread which runs the user interface makes a request to the thread associated with a particular detector. The detector thread makes a request for data to an emulated COM port on the computer which in turn uses the serial server to retrieve the requested data from the detector. The detector thread then sends a message back to the main thread with the requested data. Once the data is received, RadTrac utilizes the data to detect the existence and location of a radioactive source in space.

RERTR Fuels Research and Development

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A volume analysis of several images from the RERTR fuel plates was performed to compare the percent volume fraction of three (3) substances, fuel, interaction, and matrix. When exposed to radiation an interaction product forms at the fuel/matrix interface. A convergence study was performed to estimate the required quantity of data points to evaluate the volume fraction of each constituent. This study showed

that the desirable number of points is between 375 and 400. With this evaluated, the volume fraction program was used to acquire extensive information regarding if an image has the minimal amount of interaction. A compilation of twenty-five (25) RERTIR irradiated plates with different matrix compositions were analyzed individually, then averaged according to the plate it corresponds with. The data was evaluated to determine the final interaction percents for each plate and F3R040 had the least amount of interaction. At 14.54% interaction it showed the best matrix blend to obtain minimal interaction.

Physics

Detailed Simulations of Third Generation Time-of-Flight Neutron Powder Diffractometer, POWGEN3

Prabal Adhikari (GRINNELL COLLEGE, GRINNELL, IA 50112), Jason Hodges (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). POWGEN3, when fully constructed, will be an extremely versatile diffractometer for the study of polycrystalline materials. Its design incorporates the very intense pulsed neutron source at the Spallation Neutron Source with an innovative detector design having wide angular coverage. This will enable the collection of very large parametric data sets in only a few hours time. The aim of the research project is to accurately model the POWGEN3 instrument and setup a software suite to simulate full parametric data sets. First, the three-dimensional geometry of the detector array (300 000 pixels) was defined in a vector representation. This was combined with a Monte Carlo simulation of the instrument super-mirror neutron guide to determine the resolution function for each pixel. Separately, the neutronic performance of the top-up stream hydrogen (H_2) cryogenic moderator was fitted to analytical models (of intensity and time emission profiles). To simulate a full parametric data set, the representative crystal structure of FeSi was modeled using a first-order Grüneisen approximation for the zero pressure equation of state. From these models, the structure factors for all the diffraction reflections were calculated using FullProf over the temperature range from 20K to 1200K. This crystal structure model accounted for the change in lattice parameters and atom thermal parameters as a function of temperature. The instrument resolution functions and moderator models were then combined using a program pkf to simulate a diffraction profile for each pixel and temperature. To reduce calculation time, only the center pixel of the detector module was used in the diffraction data set simulations. In all, 8806 different pixel diffraction profiles were generated and these were focused to yield the final series of 119 instrument diffraction simulations over the entire temperature range. These data will now be used by the National Science Foundation funded software DANSE project at Michigan State University as part of the development of a new generation of neutron scattering data analysis software.

Innovative Approaches to Radiation Detection Materials: The Challenge of Lanthanum Trichloride

Corri Alexander (AMERICAN RIVER COLLEGE, CARMICHAEL, CA 95841), Dale Perry (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). The search for new scintillation materials that can both apply to and improve the many fields of radiation detection is a high priority for modern technology. Lanthanum halides are among a large list of rare earth halides that are suspected to have high potential in the field of radiation detection. Unfortunately, there is relatively little known about the physical properties of such materials, which inhibits the ability of researchers to predict materials that will scintillate. This study addresses this by experimenting with crystal formation of $LaCl_3$ doped with Gd using pulsed laser deposition. The purpose of this research is to attempt to perfect the thin film fabrication of $LaCl_3:Gd$ so that it can be analyzed and characterized for its physical properties as well its applicability as a scintillator. The obstacle to overcome is the highly hygroscopic nature of $LaCl_3$ which complicates the thin film fabrication process. There were few conclusions reached in time for this publication, as it is the first baby step in a very large project. Researchers will pick up where this team left off by continuing to analyze the thin films produced here, and apply the learned experimental process to future research on lanthanum halides.

Determination of Magnetic Field Pitch Angle Fluctuations in the Motional Stark Effect Diagnostic Edge Channel on NSTX

Marc Becchetti (UNIVERSITY OF MICHIGAN, ANN ARBOR, MI 48109), Fred Levinton (PRINCETON PLASMA PHYSICS LABORATORY, PRINCETON, NJ 08543). The Motional Stark Effect (MSE) uses the splitting and polarization of emitted light from a beam of neutral hydrogenic atoms in an electric field to measure the pitch angle of the magnetic field in confined plasmas. The results give an accurate evolution of the safety factor and current profile inside a tokamak, necessary for understanding

stability issues involved in magnetic confinement. The edge channel of the MSE diagnostic for NSTX displayed 2–3 degree fluctuations in the pitch angle occurring for a portion of the discharge. Individual discharges that displayed these characteristics were identified for a large number of test runs. By comparing data from the multipoint Thompson scattering diagnostic it was shown that the fluctuations were not endemic to discharges that displayed low signal and density. Also, short bursts of H-alpha light indicating Edge Localized Modes (ELMs) were observed on discharges without fluctuations, eliminating them as a possible source. Further data from the Charge Exchange Spectroscopy diagnostic (CHER) is required to compare excursions in radial electric field from changing poloidal flow in the plasma to the observed pitch angle fluctuations.

Heavy Ion Effects on Geomagnetic Field Line Resonances in the Earth's Magnetosphere

Tom Bird (UNIVERSITY OF WISCONSIN—MADISON, MADISON, WI 53703), Jay Johnson (PRINCETON PLASMA PHYSICS LABORATORY, PRINCETON, NJ 08543). Geomagnetic Field Line Resonances (FLRs) are an ubiquitous and important phenomena in the Earth's magnetosphere. An accurate model is developed and eigenfrequencies of higher frequency FLRs are calculated. These resonant modes are excited by various processes in the magnetosphere and solar wind. Ground based magnetometer stations as well as in situ measurements with satellites have provided a significant amount of experimental data on FLRs. Previous calculation of the eigenfrequencies of these modes has primarily used a low-frequency Magnetohydrodynamic model which is only accurate for frequencies much lower than the ion cyclotron frequency. To accurately model the interaction of these FLRs with ion-cyclotron resonances, a different model must be used. Here, an analytic model for higher frequency FLRs is developed. A dipolar magnetic field model of the magnetosphere and accurate electron number density data is used. The concentration of oxygen and helium in the magnetosphere is prescribed and the effect on higher frequency FLRs is studied. The resulting eigenvalue problem with two boundary conditions is solved using a shooting method. One boundary condition is fixed and the ODE is integrated across the domain using a Finite Difference Equation or an ODE integrator. During integration of the differential equation, an analytic continuation into the complex plane is used to avoid singularities. A multi-dimensional Newton's method is used to find the roots of the system and identify modes. Successful explanation of 1 Hz pulsations observed commonly at low latitudes is presented as a result of modes trapped between damping caused by cyclotron resonances. Future work will include a two dimensional mapping of various FLR harmonics in the equatorial plane. Pending more observations of these FLRs, future work will more accurately infer the concentration of various heavy ions in the magnetosphere.

Impact of Mg Concentration on the Donor Ionization Energy of $Zn_{(1-x)}Mg_xO:Al$ Thin Films

Evan Briggs (MIAMI UNIVERSITY, OXFORD, OH 45056), Xiaonan Li (NATIONAL RENEWABLE ENERGY LABORATORY, GOLDEN, CO 89401). $Zn_{1-x}Mg_xO:Al$ thin films are Transparent Conducting Oxide (TCO) materials with potential use in Thin Film Solar Cells. It has been shown that increasing Mg concentration in the film increases the overall band gap of the material. However, electrical properties are decreased as a result. Further insight on the mechanism of the band gap increase and electrical property decrease can help researchers better understand and control the material's properties. $Zn_{(1-x)}Mg_xO:Al$ thin films were deposited using a linear combinatorial method on a radio frequency magnetron sputtering system. This method gave samples with a gradient in Mg content. The electrical properties films were characterized through temperature dependent Hall measurement on a range of 105 to 405K. Data from the temperature dependent Hall measurement was used to calculate the donor ionization energy of the film. It was found that at low Mg concentrations, the $Zn_{(1-x)}Mg_xO:Al$ material degenerated. At higher concentration of Mg, above 7%, the donor ionization energy (ΔE_d) of the material increased with Mg concentration. It was also found that increasing the substrate temperature during deposition decreases the ionization energy of the film at a given Mg concentration. Assuming that the donor energy level of $Zn_{(1-x)}Mg_xO:Al$ does not change due to Mg concentration, the increase in donor ionization energy of the film shows that the conduction band minimum of film increases. This method of determining the donor ionization energy of a thin film can be applied to future TCOs and similar materials. $Zn_{(1-x)}Mg_xO:Al$ itself, however, would not be an ideal TCO for use as a conductive layer in Thin Film Solar Cells due to its large ionization energy. $Zn_{(1-x)}Mg_xO:Al$ may have potential in the creation of p-type ZnO films for use in semiconductor diodes.

Exploring a Complex Programmable Logic Device/Field-Programmable Gate Array-Based Triggering System for Linac Coherent Light Source

Matthew Brown (GEORGIA INSTITUTE OF TECHNOLOGY, ATLANTA, GA 30332), **Ron Akre** (SLAC NATIONAL ACCELERATOR LABORATORY, STANFORD, CA 94025). The Klystron Department at the SLAC National Accelerator Laboratory (SLAC) requires a new, more accurate triggering system in order to run tests involving the new Linac Coherent Light Source (LCLS) project. In order to meet requirements involving number of channels per test station, trigger repetition rate, delay length, pulse width and, most importantly, phase jitter, complex programmable logic devices (CPLDs) and field-programmable gate arrays (FPGAs) were investigated and tested for use in such a triggering system. Schematic-based and VHDL-based design entry both were used in programming the logic devices with functions simulating that which will be used in the test lab. The CPLD that was tested proved too small to contain the amount of logic required for a single triggering station, but the FPGA that was tested was more than adequate. Jitter was measured and calculated to be within the picosecond range as specified by the test lab. The Arcturus Coldfire processor may be used to allow communication between the FPGA and a networked computer, enabling one to adjust the various trigger delays and widths once the FPGA has already been programmed. The FPGA also possesses digital clock managers (DCMs) which may be used to finely control the phase and timing of signals at a sub-clock cycle level. It is for these reasons that an FPGA-based triggering system was recommended for use in the Klystron Department test lab.

Considerations for Optimal Polarization of ^3He Targets

Brielin Brown (UNIVERSITY OF VIRGINIA, NEWPORT NEWS, VA 23601), **Jian-Ping Chen** (THOMAS JEFFERSON NATIONAL ACCELERATOR FACILITY, NEWPORT NEWS, VA 23606).

The polarized ^3He Target at Jefferson Lab has proven to be a valuable resource for use as a polarized neutron target. So far it has been used in seven experiments, with six more scheduled to run in 2008–2009. In general, the polarized ^3He target is used as an effective neutron target for studying the fundamental structure of the nucleon, although experiments studying the structure of ^3He are also planned. The main characteristics of a polarized ^3He target are the maximum attainable number of polarized nuclei relative to total nuclei (maximum polarization), the time it takes to reach this polarization (spin-up time), and cell lifetime. Recent developments in hybrid K-Rb cell design have resulted in cells with higher polarization and shorter spin up times, but previous research shows that it could be possible to improve on this technique by operating at an optimal temperature and laser power. In this study, a spin-exchange optical pumping (SEOP) technique is used to polarize a number of hybrid cells at temperatures varying from 190–250 °C and laser powers varying from 90–150 watts. During polarization, nuclear magnetic resonance (NMR) polarimetry is used to monitor polarization during spin-up. At full polarization, electron paramagnetic resonance (EPR) polarimetry provides a calibration for the NMR signal at each temperature. Through increasing the temperature and laser power during polarization, the polarization increases by 25.4% and spin-up time decreases by 52.7%. However, it is known that at higher temperature and power the cells have a shorter lifetime. By decreasing the spin-up time of the cells and increasing their polarization, the usefulness of the target during the experiment improves in two ways: increased polarization allows the target to more effectively emulate a neutron target, while shorter spin-up times allow faster corrections of measurement losses leading to higher operational polarization.

Modeling Energetic Ion Loss in the National Spherical Torus Experiment

Joshua Burby (CORNELL UNIVERSITY, ITHACA, NY 14853), **Douglass S. Darrow** (PRINCETON PLASMA PHYSICS LABORATORY, PRINCETON, NJ 08543). A particle's guiding-center trajectory in the National Spherical Torus Experiment (NSTX) is uniquely determined by three quantities that remain constant throughout the particle's motion: canonical angular momentum, magnetic moment, and energy. We calculated these constants of motion (COM) for energetic ions bred by the neutral beams in NSTX. Our goal was to calculate the fraction of these ions that leave confinement by determining which values of the constants of motion correspond to particles with trajectories that intersect the wall of the machine. After finding a way to divide the COM phase space into a confined trajectory region and an unconfined trajectory region, we determined the beam ion loss fraction for various shots by counting the number of beam ions with COM coordinates in the unconfined region. To test this model, we used it to predict measurements taken by a fast ion loss probe mounted in NSTX. These predictions were fairly

accurate in relevant cases. The level of agreement between model and measurement suggests that the method we used should be refined further in order to increase the accuracy of the method. An accurate implementation of this method would provide a computationally efficient alternative for calculating non-collisional particle trajectories in NSTX.

The Effect of Source Rate and Water Content on the Gain Stability of GEM Foils

Adam Caccavano (UNIVERSITY OF OREGON, EUGENE, OR 97401), **Craig Woody** (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). GEM foils produced at Tech-Etch have been shown to exhibit charging up effects, observed as a gain increase in time, which can be fit to a saturating exponential. The reason for this gain increase has been attributed to an increasing electric field within the electron avalanche region due to charge accumulation on the insulator surface. The gain from triple-stacks of TE foils operating in Ar-CO₂ (70:30) with a 5.9 keV X-ray gun source (simulating ^{55}Fe), has been measured over time to better understand this transient effect, which can last anywhere from minutes to days. The foils selected for these studies were first characterized individually, where the gain vs. time and gain vs. ΔV across the foil were measured. For all measurements, the water and oxygen levels were recorded, and the gain was corrected for pressure and temperature fluctuations. Appropriate foils were then selected for a study of the effect of source rate with triple GEM stacks. It was found that higher rates lead to a faster charging up effect. Also studied was the presence of water in the gas. Once a GEM foil reaches its plateau value for gain, it takes hours to fully discharge again once high voltage is turned off. By purging the vessel with H₂O-saturated Argon, a GEM foil can be effectively "reset" to its initial gain. It is speculated that this effect is due to an increase in the surface conductivity of the insulator through adsorption of water. Rate dependent studies were also performed with higher concentrations of H₂O (~200 ppms), where it was found that a higher concentration of water leads to both a faster charge-up as well as an increased absolute gain.

Analysis of Longitudinal Beam Quality through Light Output Collection

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The current method of performing beam diagnostics in the Neutralized Drift Compression Experiment (NDCX) involves direct measurement of current from ions using a fast faraday cup (FFC). Beam diagnostics that relate to longitudinal beam properties are compression ratio and a time profile. This study used light output collection from the photons released from the collision of ions with the scintillator located inside the NDCX's target chamber as an independent method of determining longitudinal particle beam properties. Information about the beam's time profile and intensity was extracted from the images produced by the streak camera aligned with a 400-micron fiber optic that collected light released from the scintillator. Data was analyzed and compared to FFC data for agreement. Despite a low signal to noise ratio, a compression ratio adequate to determine beam time profiles such as pulse length, full width half maximum (FWHM), and shot to shot time variation was determined. Time profile information showed good agreement with FFC data. These results lead to a conclusion that with a more sophisticated experimental set up, light output collection can definitely offer an alternative independent method of doing longitudinal beam diagnostics. Having an alternative method of particle beam diagnostics allows verification of the information presented with the current method and also a check if diagnostic equipment is working properly.

Accelerating and Focusing Modes in Photonic Bandgap Fibers

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Laser-driven photonic bandgap (PBG) fibers with hollow core defects are one option for future particle accelerators. PBG fiber accelerators use an electromagnetic wave to accelerate charged particles like conventional accelerators do, but they constrain and guide the wave in a new way. Fabrication of PBG fiber accelerators is a challenge because of their small size and high length to diameter aspect ratio. There are several different facilities that can use different technologies to come close to PBG fiber dimensions. To take advantage of well-developed nanofabrication techniques for silicon, several possible silicon PBG fiber accelerating structures were designed and studied. Searches for modes that could accelerate and focus an electron beam were run in the simulation software BandSOLVE and CUDOS. Also, a model of a fiber from Incom was studied further in CUDOS. The simulated field data from CUDOS was then analysed in MATLAB

and scaled to find the maximum achievable accelerating gradient. Structures that support viable accelerating modes were indeed found in silicon. The accelerating gradients of all of the structures were found to be one to two orders of magnitude better than what is possible with present technology. Also, an electro-optical focusing mode was found in one of the silicon structures and accurately modeled as an electric sextapole.

Simultaneous Transverse and Longitudinal Measurements of the Compressed Ion Beam in the Neutralized Drift Compression Experiment

Allan Chen (UNIVERSITY OF CALIFORNIA—BERKELEY, BERKELEY, CA 94720), Peter Seidl (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720).

Experimental studies of Warm Dense Matter (WDM) heated by intense ion beams require accurate detection of the pulse duration and the transverse beam radius. Previously, the Neutralized Drift Compression Experiment (NDCX) experimenters at the Lawrence Berkeley National Laboratory used a fast Faraday cup (FFC) to measure the current waveform of the K^+ ion beam. The FFC provided a measurement of the beam current by detecting the charge on a collector plate. To determine the transverse beam profile, an alumina (Al_2O_3) scintillator was used along with a nanosecond resolution gated microchannel plate (MCP) camera to capture a time slice of the beam current density profile. Using image analysis software, ImageJ, the beam radius can be calculated from the image. Because each of these diagnostics must intercept the ion beam, simultaneous measurements on a single beam pulse was not impossible. We resolved this dilemma by using a streak camera to measure pulse width of the ion beam. We were also able to extract a current profile of the ion beam directly from its time dependent transverse optical image. An optical splitter was developed and the time history was simultaneously fed to the streak and MCP cameras. Results from this newly developed setup could be used to verify the temporal data obtained using the FFC and provided researchers with a new method for simultaneously diagnosing the transverse and axial profile of the ion beam.

Measuring Thickness Variation of Lead Foil Target from the Coulomb Sum Rule Experiment Using Gamma-Ray Attenuation

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The Coulomb Sum Rule experiment conducted at Jefferson Laboratory in 2007–2008 consisted of the bombardment of accelerated electrons onto several targets, including lead foil. In order to measure with high precision the electron scattering cross sections from the lead target, it is important to know the thickness variation of the lead target. The focus of the current project was to measure the variation in thickness of the foil through a technique called ‘gamma-ray attenuation’. This technique utilizes the absorption of gamma rays when traveling through some material and that this absorption is proportional to factors that include the thickness of the material. In this experiment, a 1.5 micro-Curie active Americium-241 gamma-ray source was chosen for its production of distinct and relatively low-energy gamma-rays (around 60000 electron volts). A Cadmium Zinc Telluride (CZT) detector was chosen to capture the gamma-ray signals. The lead target foil, however, was found to emit radiation more than 10 times stronger than the source; thus, because of lack of availability of a stronger source and due to time constraints, it was decided that a non-active foil cut from the same bulk material as the target foil would be measured instead. Data were taken for nine circular areas (1 mm in diameter) on the non-active foil. Twenty-four hour runs allowed for a statistical precision of about 0.53% for each measured gamma-ray intensity value. The variation in thickness of the foil was found to be less than $\pm 2.5\%$, with a statistical error of less than 1% for each thickness variation value. The data for variation in thickness in the substitute lead foil will allow experimenters to know what thickness variations to expect for the actual foil at the beginning of the Coulomb Sum Rule experiment. The data will also contribute to determining how much error to expect for the electron scattering cross section measurements. The gamma-ray detection setup is ready to be used for measurements on the actual target lead foil, as well as any other targets, once a stronger Americium-241 source is obtained.

Looking for Dark Matter Through Particle Collisions

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Particle physics studies suggest that dark matter particles can be produced in electron positron annihilations that lead to $Y(1S)$ formation and decay. This experiment focused on decays of the $Y(1S)$ particle to

a photon and dark matter particles, which would not be detected due to their weak to non-existent electromagnetic interactions. The “invisible” particles would thus be seen as missing energy and momentum. To separate background, insignificant events from the signal, the data was cut using several parameters that strengthened the signal and reduced the background.

Triple Gem Fluorescence X-Ray Detector

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The Gas Electron Multiplier (GEM) generates an electrical signal through the impact ionization of an ionized gas placed in an electric field. The noise-free amplification of electrons is utilized to detect X-ray fluorescence from elements in a sample nondestructively. We are using a triple GEM in order to detect minute sample concentrations in the range of 1–10 ppm. We expect that electron multiplication will provide an improved signal, compared to conventional detectors. We will be using 3 cascaded GEM's of 1–3 inch diameter. The goal is to get an amplification of electrons of about 1000–3000 at the readout. The Micromesh Gaseous Structure (MicroMegs), a different microstructure operating in a similar way to the GEM, may also be used in conjunction with a single GEM for comparison. We fabricated our GEM detector using aluminum and acrylic sheets. Following the completion of the detector we then applied voltages to both the top and bottom of the GEMs and also to the Mylar. Once all the voltages were applied, we discovered that the voltage on the Mylar was tripping around 1000 volts. We used different wires for connecting the voltages, different voltage sources and still were not getting the correct readings.

Microfabrication of Cryogenic Detectors for Cosmic Microwave Background Observation

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Cosmic Microwave Background (CMB) is an ensemble of photons that traveled for about 13.7 billion years after the last scattering event. Such photons are reaching us today with an effective temperature of 2.725K. Detection of CMB allows mapping of universe anisotropy, therefore giving insights about dark energy, believed to be responsible for the accelerating expansion of the universe. Detection of CMB is also useful for testing the Big Bang Theory. The 10 meter South Pole Telescope (SPT) built by the University of Chicago, is currently mounting a receiver for CMB detection which is missing the detector polarization component. Argonne's Material Science Division is developing and fabricating sensors for the receiver that will replace the current one in the SPT. These state-of-the-art Transition Edge Sensor (TES) cryogenic devices are based on superconductor technology which is featuring unique polarization sensitivity properties. Two TES detectors are currently under construction: Polarization Sensitive TES and Multispectral TES, whose detailed micro-fabrication processes are described in the present report. The Polarization Sensitive TES is selected to go in SPT, while the Multispectral TES is being developed as a next generation detector. Both devices consist of absorbers (antennas), a TES thermometer, and weak thermal connection between the TES thermometer and the environment, with the main difference between the two devices being in the design of the absorbers. A bilayer film deposition of molybdenum and gold on a silicon nitride/silicon wafer has been employed to control the critical temperature of the superconductor through the superconductor proximity effect. A bilayer of about 30 nm of molybdenum on 25 nm of gold was found to suppress the molybdenum transition temperature to about 450 mK, which is required for the current design of CMB receiver. Current research efforts are oriented toward improvement of thermal and optical efficiency. Since TES devices can be tuned to detect any radiation, such as X-ray, gamma ray, sub millimeter wavelength, alpha ray or terahertz, the applications for the device are many. To only mention some, TES devices can be used for astronomy, materials analysis, national security, cosmology and high energy particle physics.

*** Study of Contact Resistance in $La_{2-x}Sr_xCuO_4$ Thin-Films**

Brian Cooper (TEMPLE UNIVERSITY, PHILADELPHIA, PA 19122), Ivan Bozovic (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

Cuprate superconductors not only show promise because of their superconducting property, but under the effects of changing state variables (pressure, temperature, magnetic field, etc.) or the addition of dopants, they represent a veritable cornucopia of quantum phases (metals, insulators, Fermi liquids, etc.). $La_{2-x}Sr_xCuO_4$ (LSCO) thin films have one of the simplest crystal structures of all cuprate superconductors, but many difficulties can arise in the measurement process. One such difficulty, high electrode contact resistance, has hindered our ability to perform Hall Effect and combinatorial measurements of our samples. The contact resistances of our

gold deposited pads were of higher orders of magnitude than the samples' resistances, and this rendered all measurements inaccurate. Consequently, we have had to resort to depositing a few mono-layers of overdoped LSCO (0.3<d<0.4) on the surfaces of the films to abate high contact resistivity. Although the high electron carrier density of overdoped LSCO disrupts the creation of dead layers between gold and under-doped LSCO (d=0.15), it is a time consuming and inefficient process. Through experimentation with selective variations of oxygen annealing parameters (duration, flow rate and temperature), we were able to promote c-axis diffusion of gold or copper and simulate the aforementioned effect via a less time-consuming and arduous process. We have observed reductions in the contact resistivity of our pads from 1 to 4 orders of magnitude and our procedure has proven to be reproducible and viable over a wide range of LSCO dopings. Before this procedure can be adopted, we must prove that it is transferable to the length scale of the contacts that will actually be used in the Hall Effect and combinatorial measurements. The electrode pads used in this experiment were 1 mm by 1 mm in area, but the actual pad sizes to be used in the desired measurements are 0.3 μm by 3 μm in area, 4 orders of magnitude difference in length scale. Although the annealing conditions caused no degradation to the quality of the contacts in our experiment, there is a chance for (a,b)-axis lateral spread when this procedure is performed on a new set of samples because of the severe reduction in length scale. Unfortunately, due to the length of the internship, I cannot complete this portion of the experiment, but we are confident that by systematic adjustments to our parameters we will soon optimize the procedure.

Simulation of Dual-Readout Calorimetry

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Currently the energy resolution of hadronic calorimeters is poor compared to electromagnetic calorimeters due to various effects. One of the dominant effects limiting the resolution stems from the fact that as hadrons interact with the nuclei in the calorimeter, they can cause nuclear breakup. In this case, energy is lost to overcome the binding energy of the nucleus and this energy is undetectable. Ultimately, this leads to the fact that the energy response of a hadronic calorimeter is nonlinear and peaks below the energy of the incident hadron with a rather wide distribution. A promising idea to improve hadronic energy resolution is dual readout calorimetry. The idea of a dual readout calorimeter is based on the assumption that the ratio between the energy deposited as Cerenkov light and the energy deposited via ionization losses allows us to correct for the energy lost to nuclear breakups. We implemented such a calorimeter as a candidate to be used with one of the detector concepts for the International Linear Collider (ILC). The implementation is a total-absorption crystal calorimeter. Such a calorimeter is now technically feasible because heavy, scintillating crystals can be manufactured allowing readout of ionization losses and Cerenkov light. A candidate for the readout of this calorimeter is a recently developed silicon photomultiplier tube. This calorimeter was simulated with a Monte Carlo study using the correlation between ionization and Cerenkov light. We obtained a set of energy corrections that provide linear energy response and excellent energy resolution. These corrections do not depend on the energy of the incident particle. We studied the response of the calorimeter to single particles and will study the performance of various physics channels.

Identifying Efficient Implementation of Multi-Pixel Photon Counters into Scintillator Systems

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Photomultiplier tubes (PMTs) are the standard photo-detector in particle physics, but are unsuitable for application near a strong magnetic field or when a dense array of detectors is needed. A new type of photo-detector called a Multi-Pixel Photon Counter (MPPC) (also known as Silicon Photomultiplier) is invariant to magnetic fields and much smaller than a PMT (in this case, 3 mm x 3 mm active area). It is important to find the most effective way to use this type of detector. This experiment identifies whether MPPCs collect more light from a scintillator wrapped in mylar for internal reflection (as a PMT) or from a scintillator with a wave-shifting fiber through the center (closer to MPPC form factor) for the same energy. Sources of charged particles cause the scintillator to emit light, causing the detector to emit an electrical signal which generates histogram data representing the distribution of charge deposited into the scintillator. This experiment compares these two scintillator setups with input from two different sources, ^{90}Y beta decay in a ^{90}Sr sample and cosmic ray muons, to measure systematic error.

When the cosmic ray muons were used as a source, a scintillator-PMT system is set above the PMT-scintillator-MPPC system to establish coincidence and to filter the MPPC data based on a window of PMT values, so that only cosmic ray muons that strike nearly orthogonal to the scintillators are included. For the ^{90}Sr source, PMT and MPPC data are compared at the higher charges to differentiate the ^{90}Y beta decay from lower energy ^{90}Sr decay. It was found that the scintillator setup with the wave-shifting fiber collected 83.55 photoelectrons (p.e.) (± 1.67) compared to 30.85 p.e. (± 0.20) with the mylar when the source was cosmic ray muons and 77.88 p.e. (± 1.03) compared to 27.26 p.e. (± 1.09) when the source was ^{90}Y decay. By either measure the 2.708 to 2.858 ratio between the tests is concrete evidence that the wave-shifting fiber scintillator setup is superior. Because the wave-shifting fiber is only 2 mm in diameter, the small active windows of the SiPMs will not conflict with efficient implementation. This confirms the use of wave-shifting fibers in the current scintillator-setup in the Hall B CEBAF Large Acceptance Spectrometer (CLAS) scintillation hodoscope and the future Scintillator-setup in the Hall D Gluonic Excitations Experiment (GlueX) at Jefferson Lab.

Assembly of the Lithium Tokamak Experiment

Charles Ellison (UNIVERSITY OF COLORADO—BOULDER, CO 80309), Robert Kaita (PRINCETON PLASMA PHYSICS LABORATORY, PRINCETON, NJ 08543). The Lithium Tokamak Experiment (LTX) will explore the effects of using liquid lithium as the plasma facing component (PFC) for tokamak walls. Expected consequences include decreased recycling, increased energy confinement times, and flat electron temperature profiles. The enhanced confinement parameters and continually refreshing surface suggest liquid lithium will provide distinct advantages over previous PFC materials. The final assembly of LTX took place over the summer of 2008. While the vacuum vessel has been used in the Current Drive Experiment — Upgrade (CDX-U), the new research emphasis on a full wall (5 m²) liquid lithium PFC complicates the design and assembly. For instance, the vessel contains heated shells (400 °C) for the liquid lithium PFC. Any temperature-sensitive components had to be thermally isolated from contact with the shell segments. The potentially reactive nature of the heated lithium restricts the allowable materials within the chamber, requiring, for example, that all copper components be plated with nickel or surfaced with stainless steel. The requirements for electrical, thermal and chemical isolation for shell heaters, diagnostic sensors, and a new set of internal poloidal field coils thus limit access and introduce complexity in the assembly. The assembly process is nearing completion and will begin vacuum testing in the near future. The experiment will then begin the plasma phase in which the new diagnostics and lithium coated shells will evaluate the confinement consequences of a liquid lithium first wall in the tokamak geometry.

Determining a Heat Treatment for Bi-2212 Multifilament Round Wire

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Due to its high J_c in large background magnetic fields, Bi-2212 multifilament round wire is being developed for insert coils in accelerator magnets. The difficulty of winding Bi-2212 wire in any magnetic geometry is that it requires a wind-and-react heat treatment. Before the Superconducting Magnet Group at LBNL can begin serious fabrication and testing of magnet coils that incorporate Bi-2212, a heat treatment that produces the optimum I_c in the wire must be developed. A heat treatment in an oxygen purged environment is developed using proposed parameters where the peak temperature is varied and the ramp rates and annealing times are held constant. Heat treatments were performed before and during this study with wire from two different manufacturers referred to as company A and company B for confidentiality. A test probe was constructed to subsequently determine the I_c of each sample. Additional heat treatments with parameters specified by the National High Magnetic Field Laboratory are conducted for comparison. Test results showed that a peak temperature of 885 °C using the LBNL heat treatment resulted in an optimum I_c of 159 A for wire A. On the other hand, results showed that a peak temperature of 889 °C using the heat treatment from NHMFL resulted in an optimum I_c of 358 A for wire B. Overall, the NHMFL heat treatment provided higher critical currents and more consistent results than the LBNL heat treatment. Further heat treatments that vary parameters other than the peak temperature — such as ramp rates and annealing time — are needed in order for the Supercon Group to determine the best heat treatment for its HTS program.

Characterization of a Burle Planacon Microchannel Plate Photomultiplier Tube for Use in Picosecond Time-of-Flight Detectors

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Particle accelerators use time-of-flight (TOF) detectors to distinguish between lighter and heavier particles of the same momentum. Current TOF detectors have a timing resolution of ~100 picoseconds. A higher-precision TOF detector would allow more accurate measurement of the particles' energy in a detector such as CDF at the Fermilab Tevatron. The purpose of this project was to characterize the gain and response uniformity of the Burle Planacon microchannel plate photomultiplier tube (MCPMT) and to begin the development of a laser test stand. The characterization of the MCPMT was the beginning stage in the development of a TOF detector with a 1-picosecond resolution. A dark box containing a light-emitting diode, filter wheel and reference photomultiplier tube was used to test the MCPMT. The diode and filter wheel were used to control the amount of light used to illuminate single pixels of the MCP. The output was recorded and put into a histogramming program. The gain and number of photoelectrons were calculated from this data. The intrinsic timing resolution of the electronic components in a laser test stand has been tested. The gain mapping was not finished due to technical problems. The timing resolution of the CAMAC control module has been found to be 25 ps. The next step for this research will be characterizing the timing resolution of the MCP in a laser test stand.

Search for the Higgs Boson in Association with a Z Boson

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The Higgs boson is the last remaining undiscovered Standard Model (SM) elementary particle; its discovery would explain such phenomena as electroweak symmetry breaking and the origin of mass. At low masses ($m_h < 135$ GeV), the Higgs decays predominantly to $b\text{-}\bar{b}$, suffering from significant background at hadronic colliders. The production of an associated Z boson, which decays to a lepton-antilepton pair ($\mu^+\mu^-$ or e^+e^-), has lower background and is therefore an important channel in the search for a low-mass Higgs. This study used an integrated luminosity of 2.3 fb^{-1} of proton-antiproton collisions generated at 1.96 TeV and collected by the DØ detector at Fermilab. The analysis of the reconstructed dijet mass in the two-jet muon channel was consistent with SM prediction for background and a limit on the ZH cross-section was found to be about 40 times the SM prediction. In preparation for the next stage of analysis, transfer functions were fitted in the electron channel in order to model the detector resolution. These results are necessary for a matrix-element analysis, which convolves transfer functions with the SM matrix-element to calculate the relative probability that each event is signal or background. This technique will likely provide increased sensitivity to a Higgs signal.

Secondary Cherenkov Detectors in Q-weak

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Experiments in nuclear physics, including those at Jefferson Lab, examine nuclear structure using a high-energy beam of longitudinally polarized (classically analogous to spinning) electrons. In any precision experiment, knowing the exact characteristics of this beam and its effect on the measurement is crucial. The upcoming Q-weak experiment will extract the proton's weak charge through a high-precision measurement of the parity-violating asymmetry in elastic e-p scattering. With the data acquisition electronics phase-locked to a rapidly reversing longitudinal beam polarization, a signal proportional to the proton's weak charge can be measured. Any extraneous helicity-correlated beam modulations can potentially produce a false asymmetry that is difficult to distinguish from the relevant physics asymmetry. Of these modulations, the size and shape of the beam spot is particularly insidious. This study discusses a proposed set of Cherenkov detectors designed to measure these effects and attempts to both find the optimal geometry of the secondary Cherenkov detectors and to characterize their response to changes in beam size and position. A Gigabit European Academic Network 3 (GEANT3) based Monte Carlo simulation of the Q-weak experiment and detector setup was used to model a wide variety of dimensions for the detector. To balance needs for a high rate and high sensitivity, the significant figure of merit that was maximized was b^2r , where b is the sensitivity to beam size and r is the rate. The measured false asymmetry of the smaller bars was compared with that of the primary detectors to determine how much more efficient the secondary detectors would be at measuring this quantity. The optimal

configuration for the secondary detector was found to be 5 cm wide and 140 cm long and showed a strong response to beam size compared to the main detector. This study demonstrates the capabilities and usefulness of a secondary Cherenkov detector system in measuring beam size. A detector of this geometry would be able to measure the amount of helicity-correlated beam size modulation in 0.47% of the time previously possible. With other components measuring the effects of helicity-correlated beam position and polarization asymmetries, these bars would provide the last piece necessary for a complete set of diagnostics.

A Physics Analysis of Two Particle Flow Algorithms

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Two particle flow algorithm (PFA) software packages have been developed by the Linear Collider Detector (LCD) team at the SLAC National Accelerator Laboratory (SLAC), one by Ron Cassell, and the other by Matt Charles. These PFAs are used as the final stage of a "Full Simulation and Reconstruction" (FSR) software package that simulates the detector response of a proposed silicon detector (SiD) for the International Linear Collider (ILC). The output of these PFA packages must be tested for compatibility with appropriate physics analysis software developed here at SLAC. The two physics analysis packages used for testing the PFA output are the Linear Collider Flavor Identification (LCFI) vertexing package, and the SiD Z-Higgs-Higgs (ZHH) quark tagging analysis package. After initial compatibility issues were corrected by the authors of the PFAs, our results show that these two PFA packages are indeed compatible with the aforementioned physics analysis tools. Our results also show that the PFA packages offer physics information that is comparable to that produced by their Monte Carlo simulation counterpart. Only minor issues remain in Matt's PFA package, which must be corrected for future use with other physics analysis tools.

Analysis of Track Reconstruction and Background Using SOCRAT with GEMC-Generated Events in the CLAS12 Drift Chambers

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The Continuous Electron Beam Accelerator Facility Large Acceptance Spectrometer (CLAS) hardware and software are due for improvements in anticipation of the 12 GeV upgrade at Thomas Jefferson National Accelerator Facility (TJNAF). This includes a new drift chamber package. These drift chambers require new track reconstruction software for the tracking and parameterization of scattered electrons and other charged particles. Such software requires robust algorithms that can distinguish between background particle scattering and true electron tracks within the drift chambers. The software package, called Software for CLAS12 Reconstruction and Tracking (SOCRAT), can do just this. However, there are certain parameters within the internal functions of SOCRAT that can manipulate the track reconstruction success rate amidst various background scattering. In order to test the success rate of SOCRAT, one must know how SOCRAT deals with pure background. This is done by first creating events from a GEANT4 Monte Carlo (GEMC) for the CLAS12 setup. These events will create a certain amount of noise within the drift chambers. This noise is known as the occupancy, which is the percentage of hits on the wires coming from background. This noise was tested for consistency throughout the 3 regions of drift chambers to look for shielding design faults and electron hot spots. Testing whether SOCRAT can distinguish background from a real track is key to its success for experiments in HALL B. SOCRAT was tested using various occupancies generated by GEMC. These results might infer that certain parameters within SOCRAT are in need of tweaking or experiment-defined input. They will also aid in further design of shielding for the CLAS12 detector. The background revealed large sources of background radiation from a certain area of the beam pipe where its radius increased dramatically as it left the drift chamber region. It was found that the inconsistent thickness as the beam underwent directional changes was a large reason background particles were escaping the enclosure. This was fixed within the GEMC geometry using simple scripts. An analysis of the number of hits per cluster that SOCRAT found for correlated background reveals that there is a large peak around a certain value. This will allow SOCRAT to have an intuition of whether the cluster is from background or from a real particle. Further work can be done into the study of hits per cluster of real tracks to add more knowledge about clusters to SOCRAT's library and to further investigate the background sources in HALL B.

Development of Analysis Software for Beam Bunch Shape Monitors

Emily Gospodarczyk (ILLINOIS STATE UNIVERSITY, NORMAL, IL 61790), **Sarah Cousineau** (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). The Spallation Neutron Source (SNS) is the world's most powerful accelerator-based neutron source. The SNS facility has four major components: the hydrogen ion (H⁺) injector, the Linear Accelerator (Linac), the accumulator ring, and the mercury target where the spallation process occurs. The acceleration of the ion beam is driven by a radio-frequency (RF) linear accelerator operating at 402.5 MHz. The beam is bunched into several layers of substructure in time in order to accommodate the RF field in the accelerator and the accumulation cycle in the ring. Specifically, a 1 ms long macro-pulse of H⁺ is split into 1060 mini-pulses and the mini-pulses are further divided into micro-pulses with a separation distance of 2.4845 ns. In order to precisely tune the beam and understand the beam properties, Bunch Shape Monitors (BSMs) are placed in the Coupled Cavity Linac (CCL) to measure the longitudinal phase and energy spread of the bunch shape over the duration of a macro-pulse. The objective of the project was to develop a software package for on-the-fly analysis of BSM data in the SNS control room. The software application is a graphical user interface (GUI) coded in the Java programming language that utilizes the SNS in-house XAL programming framework. MATLAB software assisted with calculations and served as a useful benchmark for statistical computations. Preexisting software applications for other tuning devices served as models for the BSM application. The package allows the user to load multiple BSM files and select a specific file for analysis. The selected data is represented in a 2-D color plot. The user is able to view the data as a mean data plot in which the time range, the noise level, and the signal threshold are user specified. A Gaussian fit can be added to the mean data plot, and the fit results, including the center, the Gaussian sigma value, and the amplitude, are displayed in a table. The results of the entire analysis are stored in a results panel, and they can be exported to a MATLAB file. This BSM analysis software application will serve as a foundation for additional application features such as fitting the analyzed data to an accelerator beam dynamics model.

High-Pressure Xenon TPC for 0-ν Double-Beta Decay and WIMP Detection

Andre Green (UNIVERSITY OF CALIFORNIA—BERKELEY, BERKELEY, CA 94720), **Azriel Goldschmidt** (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). The Dual Purpose Underground Electroluminescent Time Projection Chamber (DUET) is a device that will be used for detecting Weakly Interacting Massive Particles — WIMPs and the detection of double beta neutrino-less decay. DUET will be a high-pressure gas scintillation drift chamber. The detector will have a cylindrical geometry and a hexagonally positioned array of PMT's (photo multipliers tubes) on both ends. The detector will also provide three-dimensional tracking of particles and excellent energy resolution. A two-dimensional track will be given by PMT readouts. The third dimension will be computed from the time between primary scintillation and secondary scintillation. The detector is modeled using the GEANT4 monte carlo program. Two primary purposes of this research were to determine the energy resolution and the acceptance in photons collected per event as a function of radial distance from the detectors central axis. Both of these quantities were calculated with monte carlo methods in the simulation. The percentage of light generated that activates the PMTs opposite the region of secondary scintillation is calculated to be ~4.7% along the central axis of the detector and falls to ~3.8% for events at the outer radius of the detector. The energy resolution with a 2 MeV electron injected into the chamber and the length and diameter equal to 150 cm is ~3.4%. This value will be improved upon in later versions of the simulation.

Magnetic Anisotropy Changes in Py/Cu/CoZr Layered Ultrathin-films

Brett Guralnick (NORTHEASTERN UNIVERSITY, BOSTON, MA 02115), **Dario Arena** (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Understanding ultrathin-film magnetic material properties will help to unlock new and innovative solutions in electronics, spintronics, and magnetic storage devices. Their interlayer dynamics can affect the high frequency response in devices such as magnetic storage devices. In layered ferromagnetic materials, a weak spin coupling can be detected using time-resolved, X-ray magnetic circular dichroism (XMCD) combined with ferromagnetic resonance (FMR). Using this method locates the magnetization where the most microwave radio frequency (RF) radiation is absorbed. One issue noticed at the Advance Photon Source (APS) is that ultrathin-film layered materials undergo magnetic

anisotropy changes when RF microwaves are applied. One theory is that the microwave radiation heats up the sample locally and energy is transferred to the sample, causing changes to the sample microstructure which re-orient the magnetic easy axis. By using circularly polarized light, it is possible to measure element specific hysteresis loops at the elemental absorption energy with the largest dichroic signal. This has been done using XMCD at beamline U4B (National Synchrotron Light Source (NSLS), Brookhaven National Laboratory). Ultrathin-film samples of permalloy (an iron-nickel alloy), copper, and cobalt zirconium were made using sputtering at Columbia University. By analyzing the Iron, Nickel and Cobalt absorption edge, a change in the coercivity and/or squareness of the hysteresis loop as the RF power is varied signifies a change in the anisotropy of the material. However, this effect was not observed at U4B when subjecting the samples to microwave power at the resonant FMR field. Two possible explanations are: (1) this phenomenon only happened in the sample at APS because there was some form of defect in the film, or (2) some small change in setup exists between APS and NSLS changing the behavior of the system. Sample variability is the most likely explanation for what was observed at APS. This investigation revealed no major anisotropy changes and, therefore, suggests that ultrathin-film samples may continue to be used in magnetic experiments without worry about changing the film properties.

Wobbler Dynamics for Heavy Ion Fusion Drivers

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The Heavy Ion Fusion Science Virtual National Laboratory is reviewing beam wobbler methods for upgrades to the Neutralized Drift Compression Experiment in addition to future inertial confinement fusion and high energy physics applications. The wobbler system will smooth the ion beam and deposit its energy uniformly about an annular region on the target, consequently mitigating the Rayleigh-Taylor (RT) instability. The wobbler's two pairs of radio frequency-driven (RF) electrode plates form this annular structure by accelerating different axial slices of the incident beam in appropriate transverse directions. A lattice of alternating-gradient quadrupole magnets will then reduce the focal size of each slice. The nonlinear system of ordinary differential equations describing the centroid and envelope dynamics through the wobbler and final focusing magnets has been derived for an elliptic beam of uniform density in axial cross-section. Multidimensional Newton methods identified electrode and lattice configurations yielding sufficient deflection and convergence. In the case of a 1 kA, 50 MeV Ar⁺ incident beam, an explicit fourth-order Runge-Kutta method was used to analyze the dynamics of an infinitesimal beam slice and estimate design parameters for deflection and transverse compression both with and without self-field effects. Leading-order results have indicated feasible requirements for the wobbler voltages and quadrupole gradients. These practicable improvements will yield higher neutron fluxes and increase fusion energy gain.

Parametric Characterization of Radio Frequency Plasma Cathode

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A plasma cathode that utilizes electron extraction from a radio frequency (rf) plasma could potentially have a longer lifetime than conventional thermionic and field emissive cathodes. If integrated with ion thrusters, this rf-plasma cathode could significantly lengthen the duration of space missions that utilize thruster propulsion. We study the electron extraction for a novel low-frequency rf-cathode in the presence of gas flow. The extracting electrode (anode) is movable and biased with respect to the conducting wall of the rf-cathode. The variable parameters of interest in the rf-cathode operation include extraction voltage, distance between anode and rf-plasma source, and gas flow. The results of varying these parameters will be presented. Previously this plasma was studied under static pressure conditions. The gas flow in this experiment is expected to increase the current because more neutral atoms are available for ionization. This should mean that more electrons could be produced for a longer amount of time. In addition we characterize the initiation of a low-pressure rf-discharge using a ferroelectric plasma source, which we also expect to increase thruster lifetime when integrated with rf-cathode technology. This characterization includes imaging, therefore much of our work includes testing and calibration of an intensified CCD by imaging a plasma globe. The ultimate goal is to optimize electron source lifetime.

*** Soil Activation around Brookhaven National Laboratory's High Energy Beam Transfer and "U" Line Beam Tunnels**

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At Brookhaven National Laboratory (BNL), the soil shielding at the High Energy Beam Transfer (HEBT) and "U" Line beam tunnels of the Alternating Gradient Synchrotron (AGS) facility contains some areas called "hot spots" that have been subjected to potentially hazardous levels of radiation. As it is BNL's responsibility to acknowledge and address any potentially harmful environmental consequences of the lab's operations, the soil radiation levels around these hot spots need to be accurately estimated so that proper safety precautions can be taken. We have run Monte Carlo simulations in which proton beams in the HEBT and "U" Line tunnels are collided with steel targets called "beam dumps". We used the three-dimensional geometry and material specifications of the future beam dump of the HEBT tunnel and the current beam dump of the "U" Line tunnel in our simulation and mapped the simulated radiation levels in the surrounding environment in two-dimensional plots. A Monte Carlo simulation program, developed at Los Alamos National Laboratory, called Monte Carlo N-Particle eXtended (MCNPX) simulated the radiation levels as a function of position based on the input data (i.e., geometry and materials) we provided. The final products are several two-dimensional plots superimposed on the blueprint of the corresponding site.

Semi-Numerical Simulations of HII Bubble Growth During Reionization

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Related to such phenomena as cosmic structure formation and the birth of the first stars, the epoch of reionization provides a segue from the largely homogeneous universe described by the cosmic microwave background spectrum to the complexity we see today. While there are significant ongoing efforts to observe reionization, simulating reionization is an important and active area of research because it allows the testing and refining of analytical models. However, the radiative transfer simulations widely used in research, while providing a good qualitative picture of reionization, are too computationally taxing for such applications as probing a significant amount of the parameter space of reionization models. In the present study, we present an original code for simulating reionization much more efficiently based on a semi-numerical method involving a new algorithm for calculating smoothed overdensities in real space, as opposed to the fast Fourier transform (FFT) procedure used in previous semi-numerical studies. Using a cross-correlation coefficient analysis, we find that our simulations are successful at reproducing the results of previous simulations to a high degree of accuracy. Furthermore, we find our simulation code to be highly efficient, with a run time of ~10–15 minutes for the 1283-sized domains we simulate on in this study, and our design using a real-space smoothing algorithm promises a significant speed-up upon transfer to a graphics processing unit (GPU).

Target Mass Corrections to Parity-Violating Deep Inelastic Scattering

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Since the 1970s, parity violating deep inelastic scattering (PVDIS)-based tests of the standard model have greatly contributed to the modern understanding of the electroweak interaction. Continued interest in PVDIS is partially motivated by ongoing attempts to improve the picture of the parton substructure of the nucleon — a goal that requires controlled extraction of parton distribution function (PDF) data from the inclusive scattering of leptons off hadron targets. It has been found previously that clean extraction of the ratio of down to up quark PDFs (d/u) for proton targets, as well as observation of more exotic higher twist and charge symmetry violation (CSV)-associated effects in the deuteron, are potentially endangered by the uncertainties associated with a range of finite- Q^2 corrections to the PVDIS lepton helicity asymmetry. Here, the inventory of corrections to the parity violating asymmetry is extended to include target mass corrections (TMCs) obtained in the conventional operator product expansion (OPE) of Georgi and Politzer, as well as a parton-level collinear factorization (CF). In particular, the focus of this study was a precise and prescription-independent estimate of the uncertainty introduced by TMCs in the parity violating asymmetry. It is found that the magnitudes of the TMCs for proton and deuteron targets are of order 2.0% at high Bjorken x (i.e., $0.6 < x < 0.8$) in both the OPE and CF prescriptions. This additional uncertainty, when combined with the previously assessed finite- Q^2 corrections, begins to potentially overshadow the experimental accessibility of the d/u signal in the proton, as well as CSV and other

effects in the deuteron at high Bjorken x and low Q^2 . These challenges must be addressed to inspire confidence in the viability of several future PVDIS experiments, including those associated with Jefferson Lab's forthcoming 12.0 GeV upgrade.

*** Quantum Teleportation of a Single-Photon Spectral State**

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Over the last fifteen years, quantum teleportation has been both theoretically and experimentally realized. Initially, the teleportation of limited aspects of a photon, e.g., polarization, were investigated, while other degrees of freedom, such as the spatial and spectral states, are currently being examined. As a step toward the ultimate goal of total teleportation of a single-photon quantum state, we consider the quantum teleportation of a single-photon spectral state. We theoretically formulate teleportation of the spectral state using a pair of spectrally entangled photons. We derive an expression for the teleportation fidelity (a measure of accuracy) in terms of the spectral amplitude of the input photon and the joint spectral amplitude of the entangled pair. We calculate the teleportation fidelity for the case of a Gaussian joint spectrum and we examine the behavior of the fidelity with respect to various parameters. We obtain expressions for the fidelity for different cases of entanglement. In the case of no entanglement, we find, as expected, that fidelity is high only when the input photon and the mediating entangled photon are coincidentally already in the same state. We are working to refine and interpret the teleportation fidelity derived when using an approximation to the joint spectral amplitude arising from spontaneous parametric down conversion (a physical mechanism for producing entangled photons). These results will allow the fidelity to be quantified with respect to the degree of spectral entanglement. Provided the teleportation fidelity is found to be sufficiently high with respect to the spectral degree of freedom, this approach to spectral teleportation will enable information to be simultaneously encoded in different degrees of freedom. Being able to encode information in the spectrum and polarization of a single photon will impact the field of quantum information science, where photons are routinely used to realize quantum communication and quantum computation protocols.

Chaperonin Protein Expression and Purification That Will Serve as a Versatile Platform for Ordered Nanoparticle Arrays

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In an attempt to bring about a more efficient energy harvesting technology as well as better and more functional bio-detection systems, we are using engineered chaperonin proteins originating from the hyperthermophilic archaeon *Sulfolobus shibatae* to pattern various types of nanoparticles, including semiconductor quantum dots and metal (gold) nanoparticles, in 2-D arrays. *S. shibatae* chaperonins are donut-like shaped proteins which self-assemble from heat-shock proteins (HSP60) in the presence of Adenosine-5'-triphosphate (ATP) and Mg^{2+} . This particular protein is extremely stable in harsh conditions, including high temperatures (up to 80 °C), low pH (pH~2) and, most importantly, can tolerate genetic manipulations. Currently, we are attempting to assemble genetic variants of the wild-type chaperonin from *S. shibatae*; however, the presence of misfolded subunits prevents crystal formation. Therefore, we are currently exploring methods for purifying protein subunits with a high yield (>90%) by setting up a state-of-the-art protein expression and purification laboratory in the newly-established Center for Functional Nanomaterials located at Brookhaven National Lab (BNL). At BNL, the approach being taken to overcome this crystal formation obstacle was to change variables in the expression process one at a time and purify small amounts of the protein with a fast protein liquid chromatography system. These small amounts were then assembled in the presence of ATP and $MgCl_2$ and the assembled protein was checked with native PAGE gels. Once the gels showed little or no presence of the unassembled subunits (misfolded protein), we assembled 2-D crystals of these chaperonins and conjugated them with water soluble quantum dots so they could be later characterized using a Scanning Transmission Electron Microscope (STEM). Our most current experimental data shows that the permuted subunits expressed well in *E. coli* and were purified well in excess of 90%. Also, the subunits modified by circular permutation assembled into double rings with efficiency similar to that of the unmodified subunits as indicated by non-denaturing gel electrophoresis. In conclusion, because the cells were not heated after they were lysed during the expression process and the cells were induced with a lower level of IPTG, we were able to modify preexisting purification protocols to give us the means to purify protein subunits with a high yield (>90%).

Analysis of Nuclei Produced from High-Energy Deep Inelastic Reaction

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The purpose of this experiment was to explore a new reaction mechanism to populate high spin states neutron-rich isotopes above the doubly-magic ^{48}Ca nucleus and isotopes around the ^{26}Mg target. Data analyzed in this paper were taken over a period of three days at the Argonne National Laboratory ATLAS accelerator using the Gammasphere, a gamma ray detector comprised of 100 Compton-suppressed, high-purity germanium (HPGe) detectors arranged in a spherical geometry. Data were taken to explore the viability of a new approach to studying neutron-rich nuclei using lighter projectile-target combinations and beam energies. The beam was ^{48}Ca at 320 MeV and the target was ^{26}Mg . Calibration with respect to energy and efficiency was carried out with known isotopes ^{152}Eu , ^{56}Co , ^{247}Am and ^{182}Ta . Online activities were identified and Doppler corrections were performed using ^{64}Cu gamma rays observed from the various rings in Gammasphere. The coincidence relationship of transitions in ^{64}Cu was analyzed and a partial level scheme in ^{64}Cu was proposed. The largest part of the data analysis process was the identification of activities, the daughters and granddaughters of the reaction products. The data were sorted into a matrix of γ - γ coincidences and a cube of γ - γ - γ coincidences with proper Doppler correction. To construct the matrix or cube, the data are sorted such that each axis corresponds to the gamma-ray energies and the points on the cube are gammas that came in coincidence with the gammas on the axes. In the case of cube, two gates can be set so that certain energies are selected and then they are projected onto the third axis so that the coincidences are evident. A level scheme for ^{64}Cu was constructed using a cube for triple gamma coincidences and RADWARE software. There are two known levels, at 159 keV and 360 keV with two gammas of 159 keV and 201 keV. Using these two known energies to set the first double gate, other gammas in coincidence with those two were identified. The strongest peaks in the subsequent double gated spectra were followed and an attempt was made to place them in the level scheme. There were 79 possible transitions to be placed from the singles spectrum. Based on the double gate set at 159 and 201 keV, 25 of those were placed in the level scheme and were arranged in such a way that resulted in 24 levels. The level scheme for ^{64}Cu was constructed.

Feasibility Study of the Measurement of Charge-Symmetry Violation Using Nucleons

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Charge Symmetry is assumed in nearly all medium and high energy interactions because of the simplification it provides by cutting the number of required quark parton distribution functions in half. However, recent experimental work indicates that this symmetry may be violated by up to several percent in certain kinematic regions. Previous work is open to interpretation as to whether flavor symmetry or charge symmetry breaking is contributing to the measured effect. The experiment examined here will isolate the charge symmetry contribution. First, the charge symmetry violation terms were mathematically isolated. Programs were written to estimate the range of charge symmetry violation expected in various kinematic regions as well as to see if an extraction of these values was possible from the format of data expected from the experiment. A Monte Carlo simulation using PYTHIA to simulate the experiment was begun, but was not finished during this program. Since the Monte Carlo programming assumes charge symmetry, a strong test of our programs would be to run them on the PYTHIA results and extract a zero for our measurement of charge symmetry.

* Installation of Muon Trigger Electronics for W-Boson Detection in the PHENIX Detector Forward Arms at the RHIC

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The origin of proton spin is one of the most fundamental unanswered questions within the Standard Model. Twenty years ago, data from deep inelastic scattering experiments demonstrated that the proton's constituent valence quarks only contributed a small fraction of the observed spin of 1/2, marking the beginning of the "proton spin puzzle." The Pioneering High-Energy Nuclear Interaction Experiment (PHENIX) detector will explore this mystery over the next 5 years by observing single spin asymmetry from W-bosons produced in spin-polarized proton-proton collisions at Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC). This first direct measurement of the proton's sea quark spin contribution requires a major modification

in the background rejection capability to the triggering system of the PHENIX muon arm. The PHENIX Muon Trigger (MuTRG) collaboration developed the MuTRG Amplifier-Discriminator Transmitter (MuTRG-ADTX) circuits to supplement the momentum selectivity of the existing triggering system in order to effectively distinguish high-momentum muons produced in the decay of W-bosons from dominant background processes. Over the past two months, we have participated in the testing process of the newly developed circuits, which has involved producing analog-to-digital interface circuits as well as the associated cables that connect them to the ADTX boards. We have also worked to develop other necessary infrastructure, which included optical cable testing, labeling of optical and low-voltage cables, bundling of all the cables and installation of the cables into the muon arm.

Silicon Detector Design Study Tracking Analysis Program Development for the International Linear Collider

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An analysis program to study the track finding ability of the Silicon Design Study's (SiD) simulation program is described. This program includes analysis of the resolution of five helical track parameters, the efficiency of the track finding, and the fake track rate. The resolution of the helix parameters is determined by comparing the results from the HelicalTrackFit class, the track finding algorithm, to the Monte-Carlo Particle (MCParticle) parameters directly calculated from the simulation. Pull distributions are used to show the residual of the different parameters over the error. The track finding efficiency is determined by taking the total number of found tracks divided by the total number of findable tracks. During simulations of $e^+e^- \rightarrow Z^0$ events the track finding efficiency was found to be $98.6 \pm 0.1\%$. A track is considered to be fake when it has a purity of less than 50%. One-thousand single Z^0 simulation events were run and of the 8825 tracks found, none were deemed to be fake tracks. Of those tracks, $96.4 \pm 0.2\%$ were found to be 100% pure.

Search for 4-Jet Decay Modes from Colored Resonances in P-Pbar Multijet Channels at the Collider Detector at Fermilab

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The results of an ongoing search for new double-dijet resonances in events with 4-jet topology at the Collider Detector at Fermilab (CDF) Run II are presented. Many models of physics beyond the Standard Model predict new massive colored bosons (colorons) decaying into streams of fundamental particles known as jets. A coloron-to-dijet resonance below 2 TeV has been ruled out, however, theorists suggest a large discovery potential at the Tevatron for coloron-to-4-jet resonances. Code was written to compare real and simulated proton-antiproton events at center of mass energy, $\sqrt{s}=1.96$ TeV. Simulations were created with Monte Carlo implementations, whereby a random number generator creates particle track data and approximates detector response. Misleading data from cosmic rays and other phenomena were removed from the samples and their effect on background were studied to eliminate bias. Good shape agreement between CDF background energy distributions and simulation was shown. Comparisons of these simulations to data show good agreement in jet multiplicity and inclusive jet transverse energy distributions. Challenges in finding the best-matched-pair of dijets were revealed by comparing a simulation of expected signal (180 GeV) with background and measuring differences in paired dijet's invariant masses. At present, no resonance has been found due to the large background significance. This investigation shows our simulations of multijet background are accurate enough to proceed with the search. However, lower background significance and higher signal sensitivity in 4-jets must be demonstrated before it will be possible to identify a resonance in CDF data.

Investigation of a Plasma Ball Using a High Speed Camera

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The physics of a plasma ball is not clearly understood. A plasma ball is a commercial "toy" in which a center electrode is charged to a high voltage and lightning-like discharges fill the ball with plasma filaments. The ball uses high voltage applied on the glass-covered center electrode (~5 kV) and capacitively coupled to the plasma filaments which fill the globe. This voltage oscillates at a frequency of ~26 kHz. In order to investigate the physics, a plasma ball was filmed with a Phantom v7.3 camera, which can operate at speeds up to 150,000 frames per second (fps) with a limit of ≈ 2 μsec exposure per frame. At 100,000 fps the filaments were only visible for ~ 5 μsec every ~ 40 μsec . This proved the plasma broke down in between every discharge.

The filaments formed in the next discharge, were in the same place as the previous filaments. This implies that the ball has a 'memory' characteristic associated with the formation of plasma filaments. When the plasma ball is first switched on, the filaments formed only after ~800 μ sec and initially had a much larger diameter. These initial discharges yielded more diffuse filaments with more chaotic behavior than when the ball reached its final plasma filament state at ~30 msec. The initial diffuse filaments did not exhibit the same 'memory' behavior as the filaments in the final state of the plasma ball. Measurements are also being made of the final filament diameter, the speed of the filament propagation and the effect of thermal gradients on the filament density. An attempt will be made to explain these results from plasma theory. Possible theoretical models include streamer-like formation, thermal condensation instability and dielectric barrier discharge instability.

An SNS Accumulator Ring Twiss Parameter Analysis Interface

Sean Lewis (INDIANA UNIVERSITY, BLOOMINGTON, IN 47404), Sarah Cousineau (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). The Spallation Neutron Source at Oak Ridge National Laboratory is on an aggressive beam power ramp-up program to reach a its target power of 1.4 megawatts. As particle beam power increases, it becomes increasingly important to understand the beam dynamics in the SNS accelerator, including beam dynamics within its accumulator ring. To describe beam transport and properties, physicists use a set of parameters, called Twiss parameters, which characterize the phase space of the beam at any point. I developed a Graphic User Interface (GUI) to conveniently compute such parameters for the beam in the SNS accumulator ring. The GUI uses file inputs from turn-by-turn measurements on Beam Position Monitors (BPMs). The Twiss parameters are computed using a recently developed model-independent analysis (MIA) technique based on singular-value decomposition. MIA has proven effective at extracting beam motion information from noisy multi-turn data and has been used successfully at the SNS in the past. These previous analyses were restricted to off-line computations done in MATLAB outside of the SNS control room. I am now implementing the same method in Java, using the extensive SNS accelerator-development package, XAL. The advantages of a Java implementation in this case are ease and flexibility when working with multiple data sets, as well as the immediate access to measurement of Twiss parameters in the control room. The GUI interface can display BPM data for user-editing and quality assurance before the analysis. Afterward, the BPM data are processed using MIA, and the GUI interface will plot the user's choice of any of the three main Twiss parameters. These advantages make the GUI valuable for tuning and operating the beam in the SNS accumulator ring.

Initialization of Magneto-Rotational Simulation of Core-Collapse Supernovae

Tony Li (CORNELL UNIVERSITY, ITHACA, NY 14853), Shizuka Akiyama (SLAC NATIONAL ACCELERATOR LABORATORY, STANFORD, CA 94025). The full mechanism behind core-collapse supernovae is currently not fully understood, as computer simulations have been unable to produce explosions for massive progenitor stars. Strong magnetic fields may play a significant role during the process by driving the stalled shock, transporting angular momentum, and possibly accounting for observed features of supernovae such as bipolar jets. However, the simulation of magneto-rotational core collapse is an inherently three-dimensional problem. In this paper, we present in detail our initialization of a fully three-dimensional core-collapse simulation, which we run using the GRMHD code COSMOS++. In our initial model, we incorporate a polytropic density distribution, a rotation profile with variable degree of differential rotation, and a poloidal magnetic field. We describe key features that we have implemented in our simulation code, including a logarithmically spaced mesh and a magnetic field inclined to the axis of rotation. In our continuing work we aim to analyze the results of a completed simulation and perform a comprehensive parameter study of magneto-rotational core collapse.

Electron Response to a Charged Particle Beam Propagating through a Background Plasma

Brendan Lyons (PRINCETON UNIVERSITY, PRINCETON, NJ 08544), Igor D. Kaganovich (PRINCETON PLASMA PHYSICS LABORATORY, PRINCETON, NJ 08543). The propagation of ion beams through background plasmas has broad applications in astrophysics, particle accelerators, and inertial confinement fusion (ICF). In particular, ion beam drivers offer an attractive alternative to high-intensity lasers for ICF. Previous analytical and numerical studies of beam propagation in cold background plasmas have demonstrated near-complete charge neutralization for long beam pulses and current neutralization for beam pulses wider than the electron skin depth. By solving Maxwell's equations in Fourier space, the self-electric and self-magnetic fields of the beam pulse

have been determined. A Matlab code was written for the purpose of visualizing the motion of the electrons in response to the passing beam. The algorithm used was inspired by the leapfrog algorithm for N-Body simulation. Visualizations of the cold background plasma case have revealed that the electron density in the beam decreases more rapidly than the current density near the beam's edge, causing a sharp increase in the electron velocity along the radial direction. This effect is more pronounced for higher beam densities and thinner beams. Results for fields and currents are discussed and shown to be consistent with previous studies. In addition, code has been written to determine the self-electric and self-magnetic field of a beam pulse propagating through a warm background plasma. Initial results reveal reduced current neutralization for higher temperatures.

Surface Treatments of Indium Tin Oxide and Exploring Amorphous Indium Zinc Oxide as a Replacement in Organic Photovoltaics

Michael Machala (KENYON COLLEGE, GAMBIER, OH 43022), Joseph Berry (NATIONAL RENEWABLE ENERGY LABORATORY, GOLDEN, CO 80401). Dispersions are tall pillars (ranging from ~10 nm to a few microns in height) found on the surface of transparent conducting indium tin oxide (ITO) that cause premature burn out in organic photovoltaics and organic light emitting diodes. We compared two common dispersion removal techniques (rubbing with a nitrile glove and brushing with a Sonicare™ toothbrush) against a novel procedure (irradiating with microwaves) using optical interference profilometry. Preliminary results suggest that microwave irradiation may be an effective, non-contact dispersion removal technique that has the potential for commercial application. Shortening or removing conducting dispersions and other surface defects will reduce the severity of hotspot formation and thus increase device performance and lifetime. To forgo dispersion removal surface treatments, amorphous indium zinc oxide (a-IZO) was tested as an alternative, dispersion-free transparent conducting oxide (TCO) with a local rms surface roughness of an order of magnitude less than that of ITO. With an efficiency of 1.25% compared to a 1.58% efficient ITO control, our initial device results indicate inverted geometry devices using unoptimized IZO with a solution-derived (sol-gel) ZnO hole-transport layer are promising. A more uniform ZnO layer was deposited via pulse laser deposition (PLD) to investigate interfacial charge transport between a-IZO and the two different ZnO layers. An increase in fill factor was observed at the cost of a decrease in the short circuit current for the PLD device, suggesting a difference in morphology of the film. Initially, the PLD ZnO performed much better, with an efficiency of 1.25%, but the solution-derived ZnO performance improved with time, eventually matching the PLD results.

Building an Improved Computer Model for Accelerator Beam Optics

Theodore Marschall (CARLETON COLLEGE, NORTHFIELD, MN 55057), Yitao T. Yan (SLAC NATIONAL ACCELERATOR LABORATORY, STANFORD, CA 94025). A method for creating a computer model for a particle accelerator is presented. The calculation of Green's functions from measured data is outlined as well as the calculation of an ideal lattice from the theoretical model of the accelerator. The variables of the ideal lattice must be fit so that the theoretical model matches the Green's functions. The program uses an iterative process to fit a large number of variables and a large matrix M until the difference between the observations and what the model calculates, b, is close to zero. In order to get the program to converge, the matrix M had to be decomposed into its eigen-modes using a singular value decomposition (SVD), and the modes which were most important for producing convergence were selected each in each iteration. Several aspects of this fitting process were investigated. A faster method for selecting the optimized truncation level of matrix M was tested, which was able to select modes faster without any significant cost on the efficiency of convergence. The efficiency of the convergence process was also tested for different methods of selecting modes and it was found that using the sizes of $\lambda_{12}u_{1Tb}$, $\lambda_{13}u_{1Tb}$ or $\lambda_{14}u_{1Tb}$ were all good methods. Progress on the application of the model to the Cornell Electron Storage Ring (CESR) is also discussed.

ITER Motional Stark Effect Calibration System Investigation

Alissa Mezzacappa (VASSAR COLLEGE, Poughkeepsie, NY 12604), Elizabeth Foley (PRINCETON PLASMA PHYSICS LABORATORY, PRINCETON, NJ 08543). In 1985, at the Geneva superpower summit, plans for the world's largest collaborative fusion effort were born. Since then, the multi-national endeavor for viable fusion power has been dubbed "ITER", Latin for "the way". One diagnostic system on ITER will be the Motional Stark Effect (MSE). The MSE system measures magnetic fields of in-vessel plasma by observing the polarization of spectral lines from a beam of neutral hydrogen atoms traveling through the plasma. In order to protect the outside area from radiation a thick shielding will be installed around the ITER vessel, thus the light for the MSE diagnostic will pass

through a labyrinth of mirrors. The first mirror will have continuous exposure to the plasma creating a variation in the polarization of the reflected light. Details for a calibration system were investigated by testing aluminum and gold mirrors at varying angles of incidence and by testing a gold mirror at varying tilt angle. Laboratory setup included a movable polarized light source, a mirror, a polarimeter and lock-in-amplifiers. Mueller matrix algebra was utilized to determine the polarization angle and the phase shift of the reflected light. Then values of phase shift and slope measured were plotted. In the final calibration system it will be important to obtain a slope of unity for the measured angles of polarization. Within the measurements of variation of angle of incidence, the aluminum mirror results showed some behavior which could be attributed to oxide coating and the gold mirror results matched expectation, displaying an ability to apply theory to understand the effect of reflection on polarized light without the presence of an oxide coating. Measurements of variation of tilt unveiled a far more complex geometry than previously assumed. These preliminary results provide a firm foundation for further investigation into the particulars of the ITER MSE calibration system.

X-Ray Diffraction Patterns of Single Au Nanoparticles

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X-ray diffraction is a critical technique for structural determination of fixed macromolecular crystals, relying on lattice periodicity to induce constructive interference of photon scattering amplitudes at angles satisfying the Bragg condition. This study investigates the application of this technique to the imaging of a single gold (Au) nanoparticle aligned within an optical trap. A rectangular prismatic Au nanoparticle of 107 atoms is probed by a 20 keV hard X-ray pulse of 106 photons and (10 μm^2) cross section to match the specifications of existing third-generation synchrotron radiation sources. The resulting diffraction pattern is considered in the small and wide angle regimes to demonstrate the applicability of this technique on all structurally relevant length scales. The response of diffraction patterns to variations in particle aspect ratio and alignment angle with respect to an incident X-ray pulse are demonstrated. Wide angle scattering resolves Ångström length scales and indicates lattice alignment sensitivity through the intermittent appearance of Bragg diffraction peaks, while small angle scattering responds to nanometer-scale alterations through the evolution of the intense scattering boundary surrounding the forward peak. Small angle scattering accounts for twenty detectable photons per X-ray pulse at optimal alignment and is present throughout all alignment angles, whereas wide angle scattering collects a maximum of four photons within narrow alignment intervals. X-ray diffraction in the small angle region is thus the best strategy for measurement of the time-evolution of dynamic particle systems with use of the stated X-ray source parameters. Adjustment of the X-ray beam cross section or number of photons per pulse may permit particle structure retrieval from either angular range of a diffraction pattern generated from one X-ray pulse, suggesting X-ray diffraction as a viable tool for analyses of nanoparticle dynamics and interparticle interactions.

Exploring Light Sources and Photocathodes for Developing an Effective Purity Monitor

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Liquid argon detectors collect signals from unbound electrons created by ionization tracks from high-energy, charged particles passing through the chamber. Contaminants in the argon jeopardize the accuracy, resolution and strength of tracks by absorbing electrons before they are collected. Purity monitors have been developed that generate electrons via the photoelectric effect and accelerate them to an anode where they are collected. The presence of contaminants is determined by comparing the number of electrons generated to that collected. Finding an efficient light source and photocathode are necessary for an effective purity monitor. Existing monitors use a flashlamp and quartz fiber as a light source. Fibers are brittle, difficult to replace and vary in transmission with length and wear. A potential new light source is an ultraviolet light emitting diode (UV LED), as they are sturdy, reliable and energy efficient. Various cathodes were tested with the fiber and lamp and compared to the signal from a 255-nm LED. A comparison was made of the LED and the UV spectrum of the lamp using a phototube, yielding a signal ratio of 3:5. The lamp was then tested on various cathodes in a vacuum, the most promising of which were gold, silver and gallium arsenide (GaAs), which gave signal ratios of 1:2:3:5. A lumped delay line and switch were used to test the LED on the cathodes. These served to provide a large current (0.6 A) to the LED in a short pulse (17 μs) without damaging it. The LED to

lamp ratio allowed us to estimate the expected signal from the LED on the cathodes, however no signal was detected. The lack of signal is believed to be due to circuitry noise and oxidation or moisture layers on the cathodes. In spite of this, gold, silver and GaAs cathodes are good candidates for new purity monitors. Further tests are needed to compare them to other cathodes. A potential improvement to the setup includes building a delay line with a larger current and shorter pulse. The most promising cathodes will be tested with the LED in argon gas and eventually in liquid argon. This study will provide a comprehensive comparison of various photocathodes with UV LEDs that may be used to build improved purity monitors for liquid argon detectors.

Magnetic Analysis & Suppression of Background Signal on an Integrating Current Transformer for Laser-Wakefield Acceleration

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Integrating Current Transformers (ICTs) are capable of providing accurate measurements of the charge in an electron bunch and have been utilized successfully in many conventional accelerators. They have also been used in laser-wake-field accelerators (LWFAs) for nearly a decade. LWFAs produce accelerating gradients 1000 times greater than convention accelerators through laser plasma interactions. Here we discuss the use of an ICT in an LWFA that employs the use of a plasma-filled capillary waveguide. When a capillary waveguide is used, the gas filling a sapphire capillary is pre-ionized by a high-voltage discharge. As a result the laser is guided through the plasma allowing for an acceleration of electrons to GeV energies in centimeters. The high voltage discharge however, creates the byproduct of background plasma, which then expands into the surrounding vacuum, through the ICT. Signals not consistent with those expected from high-energy, short electron beams, as observed in conventional accelerators are seen and have been correlated with proximity to the expanding background plasma. This paper will describe experiments on understanding this ICT behavior and techniques to suppress these spurious signals magnetically in an effort to ensure more accurate measurements of bunch charge in the future. Initial results are presented including the development of a model to predict the behavior of plasma expanding into vacuum and the removal of the discharge plasma background using permanent magnets.

*** Analysis of Feed Melting Process**

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One of the largest nuclear waste sites, the Hanford site, contains 177 underground tanks with approximately 200 000 m^3 of radioactive material from plutonium production from 1944–1987. Waste disposal is an ongoing project that requires continuing research and methodology refinement to more safely and efficiently develop the waste vitrification process. To mathematically model this process, basic properties of melter feeds, such as the heat conductivity, must be determined. To this end, a method for recording the evolution of the temperature field during feed melting has been developed. Simulated high level waste feed was placed in a large silica crucible and heated at 5 $^{\circ}\text{C}/\text{min}$ from room temperature to 1000 $^{\circ}\text{C}$. The temperature was monitored using a battery of thermocouples placed into the feed. The data collected were used to determine the heat conductivity of feeds within 200–750 $^{\circ}\text{C}$, where a quasi steady state was established; the feed became glass above approximately 750 $^{\circ}\text{C}$. The heat flux at the crucible-feed boundary was estimated based on the known heat conductivity of the crucible material and the measured temperature difference across the wall. The heat conductivity was obtained as a function of temperature for ten feeds including several duplicates. The measured value was in the region of 1 to 2 $\text{Wm}^{-1}\text{K}^{-1}$. This method for recording the evolution of the temperature field during feed melting can be used for obtaining basic characteristics needed to mathematically model the cold cap.

Through-Container Measurement of Acoustic Signatures for Classification/Discrimination of Liquid Explosives (LEs) and Precursor Threat Liquids from Non-Threat Liquids

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Work at the Pacific Northwest National Laboratory (PNNL) has demonstrated that ultrasonic property measurements can be effectively employed for the rapid and accurate classification/discrimination of liquids in small, carry-on, standard “stream-of-commerce” containers. This paper focuses on a set of laboratory measurements acquired with the PNNL prototype device as applied to several types of liquids (including threat liquids and precursor chemicals) to the manufacture of Liquid Explosives (LEs) in small commercially available plastic containers. The objective of this study was to further understand

the critical acoustic measurement discrimination/sensitivity issues associated with quantifying the effectiveness of the Container Screening Device (CSD) prototype for classifying and discriminating liquid threat materials from benign and commercially available liquids. A list of pertinent threat liquids was generated and measurements were conducted to demonstrate the CSD's ability to acquire accurate and repeatable acoustic information for effectively classifying and discriminating these liquids from non-threat liquids such as wine, whiskey, water, shampoo, etc. The device was used to measure the acoustic velocity, (the primary discriminator) and relative attenuation of 181 liquids at room temperature, while recording the key parameters that play a role in the accuracy and precision (repeatability) of the measurement. Density data were manually generated and investigated to determine the effects of an additional acoustic signature to the discrimination algorithm. This effort included a rigorous statistical evaluation (using a commercially available algorithm) of all data acquired in this study. Focusing on a set of 25 potential threat liquids and LE precursors results showed that velocity alone and velocity-attenuation simulations yielded significantly more confusions with benign liquids than with the 3-parameter simulations (velocity, attenuation, density). The addition of a density signature significantly decreased the number of confusions where the velocity-attenuation-density combination performed optimally. Overall, the performance of this portable CSD prototype is comparable to that of an advanced, controlled laboratory system in its ability to acquire, analyze and provide accurate and repeatable data. In conclusion, the addition of the density metric adds significant discrimination capability to the acoustic approach evaluated and described here.

Weak Lensing Mass Measurements of Nearby Sloan Digital Sky Survey Galaxy Clusters

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Clusters of galaxies are precise probes of cosmology, large scale structure and the physics of structure formation. To leverage this observational tool, we must first understand the relation between their most fundamental property, mass, and observable quantities such as X-ray flux from hot intracluster gas (ICM) or optical counts of member galaxies. A powerful method for measuring the masses of nearby galaxy clusters is through their induced distortion, or shear, of background galaxy shapes. This weak lensing phenomenon occurs as light rays from distant sources are bent while propagating through the cluster gravitational potential. Herein we demonstrate a method for making weak lensing measurements of galaxy clusters using data from the Sloan Digital Sky Survey (SDSS). We verify the ability to make weak lensing measurements of both individual clusters and stacked ensembles of clusters and blank fields. From the full sky imaging area of $\sim 8000 \text{ deg}^2$ we create a master catalog of background galaxies containing ~ 14 million objects. We use a Navarro, Frenk, & White (NFW) mass density profile to model the measured shear of each cluster as a function of radius. This provides best-fit estimates of (1) M200, the mass within the density contour 200 times greater than the critical density of the universe and (2) a concentration parameter related to the characteristic radius of the cluster. The Abell Catalog contains 2071 rich galaxy clusters, including line of sight components, inside our footprint. We make individual mass measurements of each, representing a roughly tenfold increasing in all weak lensing measurements to date, and demonstrate a correlation between Abell richness class and mean stacked mass. Applying our technique to the Virgo cluster at a redshift of $z=0.0038$ we measure a mass of $0.8+0.5/-0.7 \times 10^{14} h^{-1}$ solar masses, the first known weak lensing measurement of this nearby cluster. For calibration purposes we measure a subset of 38 previously studied high-mass clusters falling inside our coverage footprint. We find that the weak lensing masses agree well with masses derived via dynamical estimates. Finally, the cluster masses derived from weak lensing show a strong correlation with X-ray temperature, as expected from self similar theoretical models.

Jet Reconstruction and Software Release Validation for the Compact Muon Solenoid (CMS) at the Large Hadron Collider (LHC)

John Novak (WESTERN MICHIGAN UNIVERSITY, KALAMAZOO, MI 49008), Frank Chlebana (FERMI NATIONAL ACCELERATOR LABORATORY, BATAVIA, IL 60510). The Large Hadron Collider (LHC) will be the highest energy particle accelerator in the world when it starts up in the next year. Located near Geneva, Switzerland it will accelerate protons to almost the speed of light and collide them at energies up to 14 TeV. Collisions are studied by two detectors, one of which is the Compact Muon Solenoid (CMS). In these collisions energy becomes matter and showers of particles are produced. A "jet" is a collated set of particles which is detected as clusters of energy deposits in the detectors. Jets have properties such

as momentum, energy and position and can be generated by many different processes. Distributions of the jet properties depend not only on the physics processes but also on the detector simulation and the jet reconstruction algorithm. The objective of this project was to develop a framework for comparing and validating different releases of the simulation software. The framework has also proved to be useful for comparing similar simulations with small differences, such as different magnetic field. The jet validation code was modified to output new histograms and the binning was tuned to better display the distributions. For each CMS software release, its output, which consists of about 50 histograms, were compared against previous releases. Changes in the output of different releases were identified, the histograms were published on the internet for reference and the code modifications were committed to the code repository. Full jet simulations are slow to make and take several minutes to generate each event, so there has been a move toward using fast simulations that use parameterizations of physical processes and are orders of magnitude faster. The framework was used to compare full simulations to fast simulations and it was found that they did not agree in some aspects. It was also found that there were some unexpected changes between releases of the CMS software. The framework has made it possible to quickly check new code releases and to provide immediate feed back to simulation developers.

Thermal Conductivities of Contact Bands Used for Mirror Cooling

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The mirrors used in high-powered laser systems, such as the Free-Electron Laser (FEL), absorb energy from the beam causing their shape to change. This deformation creates problems maintaining the maximum power output, as well as keeping the beam collimated and aimed. The current method of cooling uses water or cryogenics, but the maintenance involved in mounting and installing the mirrors takes days. Metal contact bands (CB) can be used with greater convenience. Because they are built for use in electronics, the thermal conductivity, which determines how well the band conducts heat away from the optic, is unknown in this application. The goal of this project was to measure the conductivities of several CBs. A neodymium-doped yttrium aluminum garnet (Nd-YAG) laser with an outcoupling optic in a water-cooled mount was used to test the CB. The optic was encircled by the CB, which was squeezed between the optic and its mount so that it made intimate contact with both surfaces. Because of the high intracavity power, this setup heated the mirror's center and created a temperature difference across the CB. An infrared (IR) camera measured the difference, which was used to determine the thermal conductivity of the CB. This was found to be ~ 0.1 Watts/Kelvin-meters. Although this is insufficient for the CB to be used for the FEL, it can be used for lower power laser systems. Further research to find an effective system for use with higher power is promising.

Studies of the Module Alignment of the ATLAS Pixel Detector Using Simulated Cosmic Data

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The Pixel Detector (PIXEL) is the innermost tracking detector of the ATLAS experiment at the Large Hadron Collider. It is built closest to the interaction point of the two counter-rotating proton beams and its spatial resolution is essential to the accurate reconstruction of collision events. Misalignments of the PIXEL silicon wafer modules from their nominal position significantly impair the resolution. A method for assessing the relative misalignment of the modules of the three PIXEL barrel layers, based on analysis of straight line tracks, is furnished. The misalignment model assumes that the modules are rigid bodies with 6 degrees of freedom represented by 6 alignment constants. Two approaches are used to calculate the constants, both based on parametrizing residuals — departures from the expected intersections of the particle trajectory with the detector modules. In this study it is assumed that modules in the outermost barrel layer (L2) can be used as reference and the rest of the modules can be aligned with respect to L2. The residuals calculated relative to a line fitted to the clusters on L2 are expressed in terms of the alignment constants to the first order. The constants are extracted independently — by fitting histograms of the residuals (histogram-based approach) and simultaneously — by minimizing a merit function (χ^2 -based approach). Both approaches are applied to simulated cosmic data representing muons passing through the PIXEL. Only modules that contain more than 50 hits are considered for alignment. The constant sets recovered by both approaches are consistent with the true values used to generate the

simulated data. The calculated constants are used to recalculate the spatial resolution of the PIXEL, which yields improvements of up to 40% in local x and up to 3% in local y resolution. Limitations of the model, including sensitivity, effects of noise and convergence upon iteration, are also investigated. As a result, the model is considered to be a viable approach to improving the PIXEL resolution within its limitations, provided that tests with real data confirm the findings.

An Analysis of Backgrounds in the Examination of Nucleon Spin Structure at Low Q^2 (JLab E97-110)

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The Thomas Jefferson National Accelerator Facility conducts research on nuclear particles at the quark level. In Hall A, experiment E97-110 scattered polarized electrons from a glass cell filled with polarized ^3He . For this experiment, measurements were made to examine the spin structure of nucleons at low Q^2 as a test of the theoretical calculations of the generalized Gerasimov-Drell-Hearn (GDH) sum rule. Strategically placed collimators blocked electrons that scatter from the windows of the target cell. Unfortunately, electrons scattering from within the target cell may have penetrated the collimators and refracted into the detector acceptance, thereby introducing an additional background. This study implemented a two-phase analysis of this background and the consequent statistical error was conducted. First, cuts on the collimator location were reversed in order to determine the background asymmetry. Then, a Monte Carlo method was implemented to simulate background from the two-step events which pass the collimators. It was found that background was small for this experiment as a result of collimator placement. Contributions from two-step scattering processes by which some background entered the spectrometer acceptance are now better understood. The background asymmetry was found to have a similar magnitude and sign to the physics asymmetry, indicating a minimal background contribution to the asymmetry. From simulated data, cuts were made on the acceptance to remove background events. Understanding of the background contribution to the cross-section has thus been improved and better fits simulated predictions.

*** Optimization of Spontaneous Parametric Down Conversion Parameters**

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Quantum computing is a radical new method of computing, but is in early stages of development. One promising method of doing quantum computing depends on photons generated by Spontaneous Parametric Down-Conversion (SPDC), a process in which one photon is "down converted" into two photons. However, most SPDC sources produce photons that are not suitable for quantum computing: the sources are not bright enough, and their photons are correlated spectrally and spatially (i.e., entangled), which limits their usefulness. We sought to optimize parameters under which SPDC occurs, which should lead to better methods for producing photons that can be used for quantum computing. To determine the optimal parameters, I used a MATLAB program to simulate a SPDC setup that displays photon emission and collection data, plus data on detection rates and degree of entanglement. I tested several experimental arrangements to determine the degree of photon entanglement and the rate of photon detection, by adjusting parameters such as crystal length, crystal material and photon wavelength. The degree of photon entanglement was measured by the Schmidt number, which equals 1 for no entanglement and increases with entanglement. We then optimized parameters to minimize photon entanglement and maximize photon detection rates. We chose periodically poled potassium titanyl phosphate as a crystal material, because previous experiments suggest it is suitable for SPDC. To represent a typical SPDC setup, we simulated a 10-mm-long crystal down-converting 780-nm photons into pairs of 1560-nm photons. We found that the optimal beam radius was 0.023 mm, with most of the photons emitted in a Gaussian distribution with a divergence angle of 15.9 mrad; this beam can be coupled efficiently to a single-mode optical fiber. The setup resulted in a spatial Schmidt number as low as 1.6. With a photon pump bandwidth of 0.85 nm, we further reduced the spectral entanglement of collected photons, with a spectral Schmidt number of 1.1. Under these conditions, the predicted collection efficiency was 46 coincident pairs of photons per microJoule of pump. Photons produced from SPDC under these conditions will be more useful and easier to detect. The reduced entanglement and greater detection rates make it easier to control a multi-photon setup, an important development in quantum computing.

Simulating Beam Passage through the Injection Chicane of the Spallation Neutron Source

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The Spallation Neutron Source (SNS) is an accelerator-based neutron source that will become the most powerful device of its kind when full power of 1.4 MW is achieved in 2009. Such a powerful source has a correspondingly small tolerance for uncontrolled beam loss, which leads to activation of the facility and longer maintenance times. To meet radiation requirements at such high energies, only 1/10 000 of the particles can be lost due to collision with the beam pipe. According to recent measurements, the area with the worst beam loss is in the injection chicane and beam dump line. Due to a structural flaw, this region will eventually need to undergo physical modification, so it is critical to accurately track the particles' paths. Previous studies have been conducted using a piece-wise symplectic magnetic field approximation, but it is now essential to track particles with greater precision using a 3-D multipole expansion representation for the magnetic field. To achieve this, a large portion of time was devoted to coding, testing, and adding C++ modules to the new Python wrapper of the Objective Ring Beam Injection and Tracking code (pyORBIT). PyORBIT is an accelerator physics code that utilizes a Message Passing Interface (MPI) for parallel computing capabilities, which is being developed at ORNL and used by accelerator facilities worldwide. Multiple benchmarks completed in the weeks leading to the final measurements agreed well with results calculated by hand. Tracking a Gaussian distribution of particles with SNS injection parameters from the primary stripping foil to the secondary stripping foil at a kinetic energy of 1.0 GeV resulted in a physically realized position and momentum confirming code integrity. It was found that the 3-D magnetic field produced 66 mm separation between H^0 and H^- components while the piece-wise symplectic only found a 61 mm separation. This higher separation could account for a greater difficulty getting the beam to enter the dump line and the observed high losses in that region. The next logical project will be to utilize the new modules in pyORBIT for a 3-D magnetic field from the secondary foil down the dump line.

Search for a Light Higgs Boson

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The fundamental nature of mass is one of the greatest mysteries in physics. The Higgs mechanism is a theoretically appealing way to account for the different masses of elementary particles and implies the existence of a new, yet unseen particle, called the Higgs boson. We search for evidence of a light Higgs boson in the BaBar datasets collected at the SLAC National Accelerator Laboratory (SLAC). Our search is motivated by theoretical extensions to the Standard Model and anomalous events observed by the HyperCP experiment at Fermilab. By comparing Monte Carlo simulations of Higgs events and background data, we identify and optimize selection criteria that isolate Higgs events from background processes. Our analysis improves on the best existing analysis (from the CLEO Collaboration) by a factor of two.

Velocity Measurements of Free Surface Liquid Metal Flows in a Magnetic Field

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In order to study free surface liquid metal channel flow characteristics in a magnetic field for applications in fusion energy and astrophysics, a potential probe diagnostic was developed and calibrated to map the velocity profile of free-surface liquid metal channel flow and quantify the effect an applied magnetic field played in shaping the velocity profile. The setup for this experiment consists of a wide aspect ratio channel sealed from the air, with argon replacing the air in the channel, placed within an electromagnet capable of producing more than a 2000 Gauss field perpendicular to the flow. An alloy of GaInSn, liquid at room temperature, is pumped through the channel by a screw pump at a specified rate. The velocity profile is obtained by measuring the voltage across pairs of probes. Various materials were used to determine which probe material would maximize the signal from the voltage induced by the Hall effect and reduce the voltage due to thermoelectric effects. Extensive calibration was then carried out to ensure an accurate velocity measurement. After amplification and filtering this signal gives us a good measurement of the velocity of the liquid metal over the cross-section of a specific probe.

Calibration of and Preliminary Results from a Beam Coincident Neutron Detector

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A variety of dark matter and other particle detectors are either running or being designed for placement in the Main Injector Neutrino Oscillation Search (MINOS) tunnel at Fermilab. These projects require a thorough understanding of the radiation background, including background caused by the Neutrinos at the Main Injector (NuMI) beam. To this end, a BC501A liquid scintillator detector was calibrated to study the neutron and gamma events coincident with the NuMI beam. Interactions in the scintillator produce photons which a photomultiplier tube amplifies into a signal and then a digital oscilloscope creates digital pulse data from these signals. A gamma energy calibration was performed with a Cesium-137 gamma source and neutron energy calibration was performed via extrapolation from previous detectors using the same scintillator. These calibrations have an estimated uncertainty of 30%. Additionally, a separate calibration was performed to determine if a gamma ray or a neutron caused a particular event. Discriminations between gammas and neutrons was achieved by an algorithm which compares the pulse shape using the ratio of two integrals. The separation was shown to be greater than 95% efficient above 1 MeV using the Cesium-137 gamma source and a Californium-252 neutron source. The calibrated detector was placed in the MINOS tunnel and connected to a data acquisition system which also recorded a timing pulse for the NuMI beam. Events occurring in a 20 microsecond window around the appearance of the beam were recorded. Non-beam coincident data showed a neutron rate of less than 1 mHz, along with a high-energy gamma (events above 4 MeV) rate of less than 1 Hz. Beam coincident data showed a neutron rate of 3.6 Hz and a high-energy gamma rate of 45 Hz. Preliminary results suggest that this detector will be a useful tool, providing us with information on beam coincident radiation for consideration in designing experiments for the MINOS tunnel. The calibrations are seemingly accurate, as basic predictions agree with these early results. Additionally, the two weeks of preliminary data suggest that the data from this detector will provide important new information about the radiation spectrum in the tunnel and how the NuMI beam affects this spectrum.

Thermal Profile of a Physical Vapor Deposition Sputter Device

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Diamond thin films are extremely hard, thermally conductive, and resistant to chemical corrosion, making them ideal coatings for various industrial and high-tech applications. They are often chemically deposited in a chamber containing a small concentration of methane in hydrogen and a substrate heated at least to approximately 700 degrees Celsius to ensure that the end product is not merely amorphous carbon. For this experiment, physical vapor deposition was used, in which argon plasma, heated with microwaves, sputtered carbon from a negatively biased graphite target onto a 3" diameter silicon wafer substrate sitting on a height-adjustable platform. In PVD, diamond growth can occur at lower substrate temperatures, but the temperature must still be controlled. In order to measure the bulk temperature, a thermocouple was placed in the substrate holder and measurements were taken at the extremes of platform height. The temperature was found to range from approximately 250 °C at the lowest height to 550 at the highest. In addition, an optical spectrometer was used to determine the average electron temperature by measuring Ar II/Ar I intensity ratios. These temperature measurements, along with the installation of a new substrate handling system with heater, will improve future film quality by allowing for more precise control of temperature.

Centering H⁻ and H⁰ Waste Beams on the Injection Dump

Fedrick Reynolds (TENNESSEE STATE UNIVERSITY, NASHVILLE, TN 37209), Larry Longcoy (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). The Spallation Neutron Source (SNS) injects a H⁻ ion beam, stripped of its electrons, into the Accumulator Ring. H⁻ charge exchange injection is used to accumulate protons in the Ring and slam them into the Hg target to produce neutrons. The H⁻ beam encounters a primary stripping foil, which strips the H⁻ beam of its electrons. However, roughly 2% of the beam is partially stripped, or misses the foil completely. Subsequently, the Injection region is occupied by three separate beams (H⁻, H⁰ and H⁺) which are affected differently by the Injection Chicane magnets. The H⁺ beam is accumulated in the Ring while the H⁰ and H⁻ beams (waste beams) are directed to the Injection Dump (IDmp), the area that absorbs the waste beams. A secondary stripping foil in the IDmp strips the remaining electrons, yielding two

H⁺ beams. The two beams are guided by various magnets, but their different trajectories make them hard to center on the IDmp. However, using loss monitors and thermal sensors (thermocouples), it is possible to center both beams. The beams need to be centered to a tolerance of ± 20 mm. The current process to accomplish the centering works reasonably well. However, after centering the beams, one typically finds that beam losses have increased and must be corrected, which repositions the beams, possibly away from being centered. Thermocouples that surround the IDmp can be used to estimate the position of the two beams. Further, we hypothesized that it should be possible to maintain suitably low losses and center the beams using the thermocouples only. If so, it should be possible to center the beams just by adjusting magnets to balance thermocouple temperatures. To test this idea, magnets along the IDmp and High Energy Beam Transport regions were changed to balance the thermocouples. Once the thermocouples were balanced, the temperatures and magnet read-back values were recorded. SNS was in neutron production mode, so testing for the actual positions of the beams was not possible: the positions of the beams had to be determined by interpolation, instead. A ratio was then created to relate the thermocouple temperatures to the positions of the waste beams. This ratio should approximate the position of the beams. Limited data collected to date supports the hypothesis. However, additional tests are needed for more rigorous confirmation of the idea that beam centering via the thermocouples is a more practical way to focus the H⁻ and H⁰ beams on the IDmp.

An Analysis of What the International Atomic Energy Agency Can Do to Evaluate and Improve Export Control Programs Globally

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The International Atomic Energy Agency (IAEA) applies safeguards and verifies the flow of nuclear materials around the world. International nonproliferation efforts also focus on export controls to regulate where, to whom, and for what purpose items that could be used for proliferation if misused are being sent. Export controls and safeguards are linked because countries with an Additional Protocol (AP) must report certain exports to the IAEA. This information provides insight into a state's nuclear fuel cycle capacity and can help shape IAEA safeguards approach to a state. Currently, the IAEA has little capacity to judge the technical effectiveness of countries' reporting. Research was done using open source unclassified documents to look at how the IAEA could evaluate the technical effectiveness of an export control system of a particular country and assess the quality of AP reports on a country's exports. This information is important in order for the IAEA to understand the quality of its conclusions. In addition, it can help countries not only improve their export control programs but also become signers and better adhere to the AP. Although the IAEA does not have the resources to provide extensive export control support programs, it could do more to coordinate support programs funded by individual countries, verify the accuracy of reports received under the AP, and provide training both domestically and at IAEA headquarters in Vienna. By improving export controls globally, countries with AP will better adhere to their obligations, countries without AP may be able to sign, and the world as a whole will be more secure against the threat posed by weapons of mass destruction.

Probing the Jet Content of Blazars Using Approximate Methods

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The electron jet content of the blazar 0836+710 is approximated using a combination of 2005 Suzaku X-ray data and a spectral energy distribution modeled from mid 1990s data in the radio, optical, X-ray and gamma-ray bands. The unfiltered Suzaku event files were processed and then fit to a power law with a galactic absorption parameter. This generated a spectrum over a range of 0.5–40 keV and an associated spectral index. To estimate physical parameters, such as average electron energy and electron density, a single emitting zone model of the jet was adopted. This assumes that the broadband emission is due to the leptonic processes of synchrotron and inverse Compton emission seeded by ambient photons external to the jet. The calculated values of 0.14 erg cm⁻³ for the electron energy density and 12 erg cm⁻³ for the magnetic field energy density suggests equipartition in the jet and agrees with an earlier, more complicated model. Applications of this sort of analysis include improving our understanding of the blazar sequence.

Scintillation Light Yield in CF₄ Gas Due to the Passage of Highly Ionizing Particles

Matthew Rumore (WORCESTER POLYTECHNIC INSTITUTE, WORCESTER, MA 01609), Craig Woody (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Scintillation light is produced by the energy deposited by ionizing

particles in certain gases such as carbon tetrafluoride (CF_4). This process is important for the PHENIX Hadron Blind Detector (HBD) at Relativistic Heavy Ion Collider (RHIC) because scintillation light is a background to the signal being detected. We have measured the scintillation light yield in CF_4 using alpha particles emitted by an Americium-241 source. As alpha particles transverse a known distance in the gas, they deposit a given amount energy and produce scintillation light. This light is detected using a CsI coated Gas Electron Multiplier (GEM) which produces photoelectrons. The photoelectrons are amplified with a triple GEM detector and the total charge is measured using a charge sensitive preamplifier and a digital oscilloscope. The energy deposited in the gas by the alpha particle is measured using a silicon barrier detector (SBD). We have determined that the scintillation light yield in CF_4 is 272.2 photons per MeV of deposited energy over a solid angle of 4π , a quantum efficiency of $20.1 \pm 2.3\%$, and a collection efficiency of $61.3 \pm 6.6\%$.

Beam Profile Monitor at the Advanced Light Source BTS

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The Advanced Light Source (ALS), the Berkeley synchrotron light facility, is currently completing the top-off upgrade, which will increase photon flux and brightness but will also require more intensive use of the Linac and Booster, together known as the ALS injector chain. The integrated flux, brightness and operational reliability of the ALS depend directly on the quality of the electron beam in the injector chain and thus on the proper operation of all its components. We installed a beam profile monitor (BPM) in the Booster to Storage Ring transfer line (BTS) that, through measurements of the electron beam transverse profile, immediately provides feedback on beam alignment and magnet strength in the injector chain. In relativistic electron beams, the distribution of photons radiated by the electrons by any process accurately reproduces the distribution of the parent electron beam. A digital CCD camera in a diagnostic line stemming from the first bend magnet of the BTS captures images of the visible portion of radiation from the electron beam, and transfers the images to a remotely controlled computer. Two possible radiation processes for the light reaching the CCD were considered: synchrotron and diffraction radiation. Various tests were conducted to determine which type of radiation is responsible, including altering the current through various corrector magnets and quadrupoles, which produces changes in shape and deflections of the center of mass of the beam. From the analysis of these data, it is evident that the source of the light must lie in an area where no magnets reside. Thus, diffraction radiation from a circular to an elliptical vacuum chamber transition, and not synchrotron radiation, is responsible for creating the images. The BPM images are also used for their primary scope, as diagnostics for beam performance, to determine extraction timing, monitor the energy of the electron beam, control the strength in the focusing elements, and calibrate corrections to the trajectory of the beam. Thus the images produced by the BPM provide information regarding the performance of the hardware of the injector chain, giving operators a tool to maintain high beam quality.

The Helical Orbital Spectrometer Project: A Superconducting Solenoid Spectrometer

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The purpose of this research is to use nuclear reactions to measure the quantum states in nuclei based on the particle energy, distance from the target and flight time obtained from silicon. This work is carried out with the Helical Orbital Spectrometer (HELIOS) which is an instrument based on a 3-Tesla superconducting MRI magnet with a 90-cm bore. This superconducting solenoid spectrometer is used for the study of reactions in inverse kinematics, in which the target and detector are placed inside a uniform magnetic field. The spectrometer will be tested at the Argonne Tandem Linac Accelerator System (ATLAS) with stable beams and subsequently with secondary short-lived beams. Testing this new type of spectrometer involves a number of tasks in setting up the experimental equipment, detectors, electronics, and computer software for data acquisition. This effort involved assisting with setting up the cabling, HELIOS readout electronics and fabricating the required cables. To reasonably evaluate the resolution and transport properties of the spectrometer, the research team has performed a detailed study of the expected performance using Monte Carlo simulations that take into account detector size and misalignment, magnetic field, target thickness effects and detector resolution effects. The research team has also decided the benchmark reactions that can be carried out using the currently available ATLAS beams. Misalignment of beamline can make it difficult to measure the time of flight obtained from the

silicon detector. Any mistakes in the beamline adjustment might cause ineffective resolution. The various electronics and cabling were successfully assembled accordingly to minimize mistakes.

Analysis of Protein Interactions Between Receptors (Ly49 and NKG2A) for Cancer Cell Ligands (H-2K and Qa-1b)

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Cancer cells have different physical properties than normal cells, such as physical shape, expressed proteins, deformability, etc. These different physical and mechanical properties can be characterized with high sensitivity and atomic resolution by atomic force microscopy (AFM). Additionally, we can use AFM to investigate the cell surface morphology and interaction forces between molecules; both of these features are expected to help differentiate between malignant cells and normal cells. Based on the AFM application of single-molecule force spectroscopy, our goal is to devise a method for studying the mechanical interactions of proteins. Mouse receptors Ly49 and NKG2A are proteins specific to malignant cells, and mouse ligands H-2Kd and Qa-1b are corresponding ligand proteins that interact with these two receptors. The focus of this study is to better understand the adhesion-force interactions between the two receptor-ligand pairs, as well as to explore the surface morphology of cancer and normal cells. As a model system, we propose to attach a receptor protein to the AFM cantilever probe tip while the protein's corresponding ligand is fixed to a substrate. This will allow us to measure the force of attraction between the receptor protein and its corresponding ligand. Once we have measured the adhesion-force interactions of the proteins and their respective ligands, we can use these force measurements to map the surface of the cancer cells, based on the cell surface's affinity for the protein on the tip of the AFM's cantilever probe. The expected results of our experiments should permit greater insight into the kinetics of the two protein-ligand complexes and the dynamic and energetic properties of these two complexes. Furthermore, by measuring the binding forces, we can determine the protein energy landscape. A good estimation of physical parameters of the cell surface may help in designing a new anticancer strategy.

Ambient Temperature Influences on the Axion Dark Matter Experiment

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The Axion Dark Matter Experiment (ADMX), if successful in detecting and identifying axions, would potentially solve two current problems in physics. The axion is a hypothetical particle that results from the spontaneous symmetry breaking of a new symmetry proposed by Peccei-Quinn in 1979 to solve the "so-called" Strong-CP problem. In addition, because the axion has mass, it is considered a good dark matter candidate. Axions decay to photons in the presence of a magnetic field. ADMX searches for the converted photons using a microwave resonant cavity immersed in a strong magnetic field (8 T), and cooled below 4K using liquid helium. The axion mass is unknown, so the cavity frequency must be swept. Given the large range to cover, it is very important that data is taken with a high duty cycle. The system was crashing frequently in May and June of 2008. It was hypothesized that the system crashes were related to the ambient temperature. Unfortunately the ambient temperature was not logged; however, a log was kept of the resistance of the magnet current leads. Comparing the cable resistance to the Lawrence Livermore National Laboratory weather data for the same period revealed that it was indeed a proxy for ambient temperature. This data confirmed that the system crashes occurred at high ambient temperatures. Ambient temperature monitoring was added to the system, and experimenters are now alerted at times when the system is at risk of crashing, a safeguard that improves project reliability.

* Construction of an Entanglement Source for a Quantum Fence

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The focus of this study is to investigate the behavior of a quantum-enhanced security system, or "quantum fence", by constructing an entangled photon source and verifying the physical nature of the polarization entangled state. The unique characteristics of the polarization entangled state suggest that a quantum fence will be impervious to undetected intrusion. An effective quantum fence could have numerous applications in quantum computing, particularly in the areas of cryptography and security. I used a titanium-sapphire laser to generate a single-mode Gaussian beam. This beam was

altered through a process called second harmonic generation (SHG), which results in an Ultraviolet (UV) beam. The entangled photons are generated through type II spontaneous parametric down conversion, which occurs when the UV beam is focused on a periodically poled potassium titanyl phosphate crystal (PPKTP). The entangled photons pass through a time delay to remove identifying characteristics. Finally, the entanglement fidelity of the photons is determined by measuring polarization correlation. We expect to find that, in a pair of entangled photons, the polarization correlation is disrupted when a single photon is replaced by a doppelganger photon. The entanglement of the original pair of photons prevents a doppelganger photon from being introduced into the system. The results, illustrated with a coincidence correlation graph, are consistent with the characteristics of the polarization entangled state described by the rules of quantum mechanics. I conclude that entanglement could be used to complement security systems that are based on the transmission of optical signals.

*** Project Mixed Apparatus Radio-Wave Investigation of Atmospheric Cosmic Rays of High Ionization**

Reamonn Soto (TALLAHASSEE COMMUNITY COLLEGE, TALLAHASSEE, FL 32303), **Helio Takai** (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Project MARIACHI (Mixed Apparatus Radio-wave Investigation of Atmospheric Cosmic-rays of High Ionization) is an ongoing research effort that includes the collaboration of Brookhaven National Laboratory, Long Island high schools and universities such as Stony Brook University and Suffolk County Community College. We seek to validate radar detection as an inexpensive tool to detect Ultra High Energy Cosmic Rays ($E > 1020$ eV) over an area of 2500 km^2 and to search for new techniques for the detection of Ultra High Energy Cosmic Rays (UHECRs). The detection of UHECRs has commonly been accomplished by detection of the particles from air showers, ground arrays, or by way of detection of the light produced by ionization in the atmosphere from Cherenkov radiation. MARIACHI is an innovative concept that will explore the detection of UHECRs by bi-static radar using VHF transmitters. This method will inexpensively and efficiently enable scientists to explore the physics of cosmic rays, their correlation with atmospheric phenomena, cloud formations and lightning triggers, as well as methods of probing the higher atmospheres and postulating questions that include where they are coming from and what kind of source is producing these cosmic rays. Using PVC pipe, coaxial connector, coaxial cable, a farad magnet and two aluminum cylindrical rods 1.07 m long each, I've constructed a dipole antenna that will be used to detect UHECRs at a frequency of 67.26 MHz . Upon completion of the antenna, I used a frequency analyzer to measure the Standard Wave Ratio (SWR) of the antenna to discover a value of 1.2 . From the SWR value, the antenna is efficient for use at the Brookhaven National Laboratory. This antenna is currently being used to detect meteors by feeding a coaxial cable from the antenna to a PRC-1000 receiver that demodulates the signal. A personal computer is connected to the receiver via sound card and uses Spectrum Lab software to collect data of High Energy events in the atmosphere at a radius of 2500 km^2 . This antenna will be installed at my house in Tallahassee, Florida to continue the gathering of data in a different area of the atmosphere. This data will then be compared to that collected at Brookhaven National Laboratory to determine any atmospheric correlation.

Search for Exotic Hadrons

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In the Quark Model (QM) of hadrons, all sub-nuclear particles are made of two or three quarks. The Quantum Chromodynamics (QCD) theory describes the composition of hadrons, but it is not limited to these two configurations. Hadrons composed of greater numbers of quarks have been predicted; of particular interest is the pentaquark, or Θ (1540), consisting of five quarks and having positive strangeness. Its existence, however, is controversial: two previous experiments at Thomas Jefferson National Accelerator Facility's Continuous Electron Beam Accelerator Facility (CEBAF) reported scant evidence for the Θ (1540). A recently completed experiment, g12, has significantly improved statistics over the earlier experiments due in part to a higher beam flux. However, because background increases quadratically with beam flux, errors in particle identification are a serious problem, particularly when looking for kaons which are produced in the decay of many particles including the Θ (1540). The focus of this research is to correctly identify kaons in preparation for Θ (1540) identification. Well-calibrated data was selected and cuts created based on the measured time difference between two detectors and the momentum of detected particles. These cuts, including one selecting the energy of the photon, were applied to the data. Currently, the f meson and the $K^*(892)$, well-

established resonances which decay to kaons, have been identified in spite of the high flux. More work is needed before conclusions can be made regarding the Θ (1540) because the current data set has not yet been fully calibrated. However, analysis of the data is making good progress, as the identification of kaons is crucial to the detection of the Θ (1540).

Waiting Points in Nova and X-Ray Burst Nucleosynthesis

Tomomi Sunayama (KNOX COLLEGE, GALESBURG, IL 61401), **Michael S. Smith** (OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN 37831). Stellar explosions are the most energetic events in the universe and synthesize the elements that make life possible. Some explosions are driven by sequences of thermonuclear reactions. Novae and X-ray bursts are driven by the rp-process, a reaction sequence that primarily involves proton capture reactions interspersed with radioactive decays. The process occurs at very high temperatures and densities. There are many uncertainties about the reaction "flow" in the rp-process, which in general fuses protons with medium mass nuclei to form heavier nuclei. One way to more thoroughly understand this process is to better determine the reactions involving waiting point nuclei. Waiting points are nuclei in the reaction path that interrupt the nuclear flow towards heavier nuclei, affecting the final abundance of the elements and energy generation rates in the explosion. They are so named because they typically have little flow through the proton capture reaction, a long lifetime against radioactive decay and the flow has to "wait" for the long decay before heavier nuclei are synthesized. There is, unfortunately, no systematic and quantitative definition of rp-process waiting points and their identification is not straightforward. A variety of criteria have been sporadically applied in the literature to determine waiting points. These criteria have included the energy release in proton capture, the radioactive decay lifetime, among others. In this project, the first set of quantitative criteria for waiting points in rp-process have been devised, written into a FORTRAN program, and utilized to search for waiting points in simulations of nova explosions and X-ray bursts. These searches have verified a number of waiting points that have previously been identified in the literature, found some new waiting points, and shown that some nuclei are not waiting points as previously speculated. This code has additionally been incorporated into the Computational Infrastructure for Nuclear Astrophysics, a suite of nuclear astrophysics codes available online at nucastrodata.org. Researchers from around the world can use this new code to specify a simulation, a time window, and values of parameters that define waiting points and let the system determine which nuclei satisfy these criteria. The first utilization of this quick, reproducible, quantitative method to determine waiting points on a number of novae and X-ray burst simulations will be presented.

Light Sources and Photocathodes for the Liquid Argon Time Projection Chamber

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Neutrino interactions can be studied in liquid argon using a time projection chamber (TPC). Charged particles produced in the interactions ionize the liquid argon and the resulting free electrons can be made to drift towards the wires of the TPC by an applied electric field, generally $200\text{--}500 \text{ V/cm}$. Molecules such as water and oxygen can be detrimental to the tracking that takes place in the TPC by absorbing the electrons before they get to the wires. A purity monitor detects possible contaminants in the liquid argon. A light source shines upon a photocathode, which gives off electrons by the photoelectric effect. The electrons travel to the anode where they are collected. The argon is inferred to be pure if the number of electrons generated at the photocathode is the same as the number collected at the anode. Effective light sources and photocathodes are necessary parts of a purity monitor. Existing purity monitors contain a flashlamp and a fiber as the light source. The fiber is brittle and difficult to replace in the purity monitor, however, so ultraviolet light-emitting diodes (LEDs) were investigated as an alternative light source. A number of different photocathodes were all tested in vacuum with the flashlamp. The fiber and flashlamp were placed with a vacuum photodiode and light was pulsed at various intensities under different conditions, including fiber length, temperature, and testing duration. The output voltage measured from the vacuum photodiode was linear as light intensity increased. The transmittance of the fiber decreased as the fiber's length increased. The temperature of the fiber did not have a significant effect on the output voltage in the phototube. After being pulsed for 16 consecutive hours at a frequency of 1 Hz , the fiber showed no significant difference in its output signal from the previous day. An LED emitting light at 355 nm and one at 255 nm were tested in the same manner as the phototube. These wavelengths were chosen

because the work functions of the photocathodes fit these wavelengths well. The 355 nm LED emits more-intense light than the 255 nm LED, though the light emitted by the latter is more energetic. Only the gallium arsenide produced an acceptable signal for use in the purity monitor; other photocathodes produced very weak signals. Gallium arsenide is recommended to be the photocathode in the purity monitor. The best cathodes will be tested in argon gas before they are implemented in a purity monitor.

Studies of the Module Alignment of the ATLAS Pixel Detector Using Simulated Cosmic Data

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The Pixel Detector (PIXEL) is the innermost tracking detector of the ATLAS experiment at the Large Hadron Collider. It is built closest to the interaction point of the two counter-rotating proton beams and its spatial resolution is essential to the accurate reconstruction of collision events. Misalignments of the PIXEL silicon wafer modules from their nominal position significantly impair the resolution. A method for assessing the relative misalignment of the modules of the three PIXEL barrel layers, based on analysis of straight line tracks, is furnished. The misalignment model assumes that the modules are rigid bodies with 6 degrees of freedom represented by 6 alignment constants. Two approaches are used to calculate the constants, both based on parametrizing residuals — departures from the expected intersections of the particle trajectory with the detector modules. In this study it is assumed that modules in the outermost barrel layer (L2) can be used as reference and the rest of the modules can be aligned with respect to L2. The residuals calculated relative to a line fitted to the clusters on L2 are expressed in terms of the alignment constants to the first order. The constants are extracted independently — by fitting histograms of the residuals (histogram-based approach) and simultaneously — by minimizing a merit function (χ^2 -based approach). Both approaches are applied to simulated cosmic data representing muons passing through the PIXEL. Only modules that contain more than 50 hits are considered for alignment. The constant sets recovered by both approaches are consistent with the true values used to generate the simulated data. The calculated constants are used to recalculate the spatial resolution of the PIXEL, which yields improvements of up to 40% in local x and up to 3% in local y resolution. Limitations of the model, including sensitivity, effects of noise and convergence upon iteration, are also investigated. As a result, the model is considered to be a viable approach to improving the PIXEL resolution within its limitations, provided that tests with real data confirm the findings.

A Bio-Inspired Approach to Tip-Based Nanomanufacturing

Delan Tai (UNIVERSITY OF CALIFORNIA—BERKELEY, BERKELEY, CA 94704), Jim Deyoreo (LAWRENCE BERKELEY NATIONAL LABORATORY, BERKELEY, CA 94720). The Coccolithophore and Mollusk are two organisms that are able to create intricate architectures of inorganic nanomaterial far more complex than current synthetic crystallization techniques allow. J. J. De Yoreo and S. W. Chung at Lawrence Berkeley National Laboratory seek to incorporate these biomineralization processes into the fabrication of nanowires and nanodots. Developing the means of growing elaborate nanostructures would have a vast application in allowing for complex nanomachines, making electronics more efficient, providing countless avenues for new technologies to develop, while simultaneously reducing production costs. This paper, rooted heavily in De Yoreo's publications on crystal growth, will cover nucleation and growth kinetics of crystallization and how organisms might apply these processes in conducting biomineralization. Based on three key principles of biomineralization, De Yoreo's research incorporates the crystallization of various inorganic materials into nanostructures using templates. As in the production of the Mollusk's aragonite nacre tablets, biomolecular templates are used to initiate and orient the growth of inorganic materials. The template consists of a gold substrate that is functionalized with alkanethiol molecules harboring reactive maleimide end groups. DNA primer is chemically anchored to the maleimide terminated self-assembled monolayer (SAM) through a thermally driven Diels-Alder cycloaddition reaction. This DNA primer allows for functional specificity when binding with a wide range of RNA mediators that are selected for compatibility with a specific inorganic material. The material growth is confined to the pattern by methyl-terminated polyethylene glycol (PEG) resists which are taller than the RNA mediators, providing chemo-physical guardrails for the nanostructure to grow between. Previous research by Chung and De Yoreo has already established the use of RNA mediators for hexagonal palladium (Pd) nanoplate growth, as well as affinity templates for controlled formation of cowpea mosaic virus (CPMV) and tobacco mosaic virus (TMV) disks.

Ongoing research is directed towards demonstrating the feasibility of bio-inspired fabrication of nanomaterials via novel biomolecular templates.

Design of New Dusty Plasma Apparatus to View Three Dimensional Particle Dynamics of Fluorescent Dust Clouds

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Particles suspended in plasmas are both contamination in industrial plasmas and a primary interstellar medium component, including structures such as planetary rings and comet tails. Typically, dusty plasma behavior in the laboratory is studied by laser scattering techniques that provide two dimensional dust cloud images. However, the three dimensional (3-D) structure of the dust cloud is essential to understand the waves, group dynamics and stabilities of the cloud. Techniques used to study this 3-D structure include stereoscopic particle image velocimetry, rapid laser scanning and ultraviolet (UV) illumination. UV illumination is a simpler technique; previous UV experiments with fluorescent dust have shown that the cloud moves ~2 mm towards the light source and begins rotating clockwise with speeds of 3 mm/s. Translational and rotational velocities of fluorescent dust particles are a function of UV intensity. A new argon DC glow discharge experiment was designed to better view the 3-D aspects of fluorescent dust. The 13.25" vacuum chamber has two 8" window ports for charge coupled device cameras, one in the horizontal plane and one viewing from above, two additional 8" window ports transverse to the plasma for laser or UV light illumination of the dust cloud, and a diagnostic probe port. Different electrodes — including mesh and ring — will be tested in the chamber to determine which one allows for optimal viewing and stable plasmas, which create stable dust clouds. Results from observations and imaging will be included. Future research will include study of the dust dynamics as a function of UV light and plasma parameters.

Improving Power Supply Monitoring Systems for the Collider Detector at Fermilab

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The Collider Detector at Fermilab (CDF) depends on properly functioning data acquisition electronics to collect reliable data from the proton/antiproton collisions occurring in the Tevatron. The electronics are powered by low-voltage power supplies, which are constantly monitored to ensure this data is valid. This monitoring system is called Voltman and utilizes a local database as well as an iFix database. These databases are accessed via a second program through a web page interface to view voltage histories. During the changes CDF has undergone for Run II and routine maintenance, these programs and databases have not been kept up to date, leaving a number of power supplies out of the monitoring system and several of the options for data retrieval on the web interface unusable, causing a major loss in time when a power supply encounters a voltage trip condition. To correct for this, time was taken to examine the power supplies for monitoring connections and editing the databases to accurately reflect the observed connections. After updating the databases, the web page was run through a series of tests to locate functional errors. The program was then analyzed for broken code in the areas responsible for the execution of the erroneous routines. Once identified, the offending lines of code were corrected or replaced. The remaining errors in the program were corrected by rewriting subroutines to be compatible with the upgrades made to the system. The resulting program provides the CDF control room with all of the necessary tools to quickly and correctly identify faulty power supplies so they can be repaired and normal data taking can resume, saving valuable time and data once lost due to an inefficient monitoring program.

Target Drive System in the Helical Orbital Spectrometer

Adam Vann (ELMHURST COLLEGE, ELMHURST, IL 60126), Dr. Birger Back (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439).

The Helical Orbital Spectrometer (HELIOS) is being developed for the purpose of studying reactions in inverse kinematics. The use of this detector for short lived nuclei will greatly increase resolution and particle identification. The magnet in HELIOS is a 90-cm bore superconducting magnetic resonance imaging (MRI) magnet. Particle identification comes from the unique property of the magnetic field that causes charged particles to travel in helical orbits. The first tests for HELIOS are tentatively scheduled for summer 2008 at the Argonne Tandem Linear Accelerator at Argonne National Laboratory. Before HELIOS can be used in experiments the main chamber of the MRI magnet must be converted into a spectrometer. One component to this conversion

is the addition of a target holder. This target holder is aligned using a telescope and is locked into position inside the main chamber of HELIOS. Each target is around 1 cm in radius and the beam spot is 1 mm in radius requiring precise alignment. The main chamber of HELIOS is in vacuum during experiments. The target holder houses nine targets and is able to rotate by means of a series of gears and a stepper motor mounted outside the chamber. The computer program LabVIEW is used to communicate with the stepper motor and an encoder to drive and record position of the target holder. The targets are located 4 degrees apart from each other so the stepper motor is capable of 32 degrees of rotation and is able to take 222 steps between each target. This configuration allows the target holder to rotate smoothly and have an accurate computer recording of its position inside the chamber.

Single Top Quark Combination Using Bayesian Neural Networks

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Top quarks were discovered at the Fermilab Tevatron proton-antiproton collider in 1995. They were first observed in pair production mode (top-antitop quark events) involving strong interactions. But the Standard Model (SM) of particle physics also predicts the production of single top quarks through the electroweak exchange of a W boson. The dominant single top production modes at the Tevatron energies are through s-channel exchange ($q \text{ anti-}q' \rightarrow W^* \rightarrow tb$) and t-channel exchange ($qg \rightarrow W^* b^* \rightarrow tbq$) with a total predicted cross section of 2.86 ± 0.33 pb at the top quark mass of 175 GeV. An observation of single top production would provide a direct measurement of the Cabibbo-Kobayashi-Maskawa (CKM) matrix element, V_{tb} , and top quark polarization, in addition to probing possible new physics in the top quark sector. Due to their smaller production cross sections and larger backgrounds compared to top quark pair production, single top quarks have not been observed yet. Evidence of their production at 3 standard deviation (σ) significance has been reported by both the DØ and CDF experiments at Fermilab at a center-of-mass energy of 1.96 TeV. At DØ, three advanced multivariate techniques were used to search for single top quarks in 0.9 fb^{-1} of data. These were Decision Trees (DT), Matrix Elements (ME), and Bayesian Neural Networks (BNN). Here we combine the results from the above three analyses by applying a second level of BNN and determine the sensitivity of our analysis under a hypothetical scenario that data agrees with SM prediction. With this assumption, the new BNN combination yields an expected measurement of the single top cross section $\sigma_{(s+t)} = 2.86 \pm 1.06$ pb. This agrees well with the SM prediction of $\sigma_{SM} = 2.86$ pb and corresponds to an expected significance of 2.71σ , which is 18% better than that obtained from a simple weighted combination of the three analyses using the BLUE (Best Linear Unbiased Estimate) method. The current analysis therefore represents a substantial improvement over previous approaches in extracting the small single top quark signals from the large, overlapping backgrounds.

Alternative Fusion Processes in Population III Stars

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The first generation of stars after the big bang may have had very different characteristics from the stars of today's universe. Population III stars, as they are called, were on the order of 100 solar masses and reflective of big bang abundances. The evolution and fusion processes of Population III star hold the key to understanding the beginnings of chemical evolution in our universe. Without metal catalysts, these early stars used the triple alpha process to create the heavy element catalysts before beginning steady hydrogen burning. The alternative fusion processes that may bypass the triple alpha process are of great interest because of the possibility of earlier hydrogen burning and lower necessary temperatures and pressures in the stellar interior to create the heavier elements. The goal of this project is to find the significance of these alternative fusion processes in stellar evolution. To do this, a model of the stellar interior was developed, assuming ideal gas, spherical symmetry, constant mass, and hydrostatic and thermal equilibria. The temperature, pressure and density were computed throughout the star as functions of radius. The star was modeled at equilibrium by computing the relation between heavy element abundances and central temperature. The elements accounted for are hydrogen, helium and the metals (carbon, nitrogen and oxygen). The next step in further work will be to model the evolution of the star up to the beginning of stable hydrogen burning, computing the changes of composition due to nuclear reactions. The reaction rates for alternative fusion processes, which are currently being researched at the Argonne Tandem-Linac Accelerator System facility, will also ultimately be

included to determine their effects. By varying the reaction rates, the sensitivity of the evolutionary process to these assumed rates can be determined.

B⁰ Meson Reconstruction through the J/ψ Decay Channel with the Heavy Flavor Tracker at STAR

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The Solenoidal Tracker at RHIC (STAR) is an ongoing experiment at the Relativistic Heavy Ion Collider (RHIC) located at Brookhaven National Laboratory. Its goals are to observe and study the characteristics of the quark-gluon plasma produced by nuclear collisions. The Heavy Flavor Tracker (HFT) is a new high-resolution vertex detector that has been proposed by STAR. The HFT will allow high-resolution tracking of charged particles, enabling the identification of particles containing charm and bottom quarks that decay hundreds of microns from the primary interaction vertex. The $B^0 \rightarrow J/\psi X$ and $J/\psi \rightarrow e^+e^-$ decay channels form a good candidate for B⁰ meson detection due to the presence of the dielectron pair generated at a large distance from the primary vertex. Reconstruction of B⁰ events mixed with Au-Au 200 GeV events was performed with HIJING, GEANT and the STAR software library. We will show preliminary results on how well the HFT can be used to distinguish prompt J/ψ from B⁰ decay J/ψ.

Magnetometry Development for a Ra-225 EDM Experiment

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It is believed by many physicists that the violation of time-reversal symmetry holds the key to physics beyond the Standard Model. One proposed way to test for this violation is by looking for a permanent electric dipole moment, the existence of which would require both parity and time-reversal symmetry violation. In the past experiments have been carried out using Hg-199, setting an upper limit on the dipole moment. A future experiment using Ra-225 is expected to push this limit within the range of values predicted by certain super symmetric models and thereby provide an important test of their legitimacy. Such an experiment as this requires magnetometers sensitive to magnetic fields on the scale of $10 \text{ nG Hz}^{-1/2}$. Such sensitivities have been achieved and exceeded in the past by exploiting the non-linear Faraday Effect. I am working to replicate such a setup, carrying out preliminary work on rubidium atoms while simultaneously working to build the coil necessary for the radium experiment. Code was written to determine optimal coil placement in order to minimize the magnetic field variation over the extent of the radium cell and the coil itself is soon to be constructed.

Photomultiplier Tube Magnetic Shielding Analysis for the CLAS12 Central Time of Flight Counter

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Photomultiplier tubes (PMTs) are used to significantly increase the signal received from a photon source in many experiments; however, their performance diminishes dramatically within high magnetic fields. This project focuses on the Central Time of Flight (CTOF) counter in the Continuous Electron Beam Accelerator Facility Large Acceptance Spectrometer at 12 GeV (CLAS12) in Hall B at the Thomas Jefferson National Accelerator Facility. In the proposed design, downstream PMTs will operate under an external magnetic field up to 1500 Gauss, while upstream PMTs will operate in an external magnetic field ranging from 400–1000 Gauss. The Hamamatsu H8500 metal channel PMT and R2083 dynode PMT are both under consideration for the CTOF counter. The R2083 cannot operate in magnetic fields in excess of 0.1 Gauss, while the H8500 is capable of operating in magnetic fields up to 200 Gauss. The purpose of this study is to design and test appropriate magnetic shielding for reducing the magnetic field to within these tolerances and to determine an appropriate PMT for use upstream and downstream in the CTOF counter. Using the POISSON Superfish computer modeling software package, magnetic shielding was designed and tested at varying lengths, thicknesses and with various combinations of ferromagnetic materials, namely iron, CO-NETIC, NETIC, and hiperma49. The data suggests that the H8500 may be a viable candidate; with a single 21 mm thick iron shield, the H8500 is capable of withstanding magnetic fields up to 2500 Gauss in the downstream portion. With a slight modification to the current design for the upstream PMT, it will be possible to reduce an external magnetic field of 1000 Gauss to within tolerances using an iron shield with a thickness of 6 mm. It was also shown that it is possible to use the R2083 in the downstream region of the CTOF counter with a new method of dynamic magnetic shielding, involving a correction coil that

is currently being tested; using a dynamic tapered shield design with an optimized length and thickness, the magnetic field can be reduced from 1 000 Gauss to less than 0.1 Gauss. These findings will influence the determination of which model of PMT and the size and shape of magnetic shielding to be used in the CTOF counter of the CLAS12 detector.

Characterization of the Magnetic Field of a Large Bore Superconducting Solenoid Magnet

Jack Winkelbauer (WESTERN MICHIGAN UNIVERSITY, KALAMAZOO, MI 49008), **Birger Back** (ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439). The Helical Orbit Spectrometer (HELIOS) is a new type of light-charged particle spectrometer, designed to study inverse kinematic nuclear reactions with unstable beams. HELIOS is based around a 3 T superconducting solenoid with the magnetic axis aligned with the beam axis. The ejected light nuclei undergo helical motion, transporting them from the target to a hollow array of silicon detectors. The heavy recoil nuclei scatter at small angles in the forward direction. HELIOS will require heavy recoil detection. Possibilities for recoil detection include an ionization chamber or an annular silicon detector. The details of a full three dimensional field map measured during fall of 2007 have been analyzed and incorporated into the existing Monte Carlo simulations. These simulations have been used to investigate the transport properties of the HELIOS spectrometer for the heavy recoil nuclei. The acceptance of these recoil detection methods, as well as details on the placement and operation of a HELIOS recoil detector will be presented. Several important results have been shown in this project. First, including the non-uniformities of the real magnetic field does not seem to cause problems for measurements using HELIOS. Next, target effects don't seem to cause any problems for the detection of heavy recoil nuclei in the $d(^{132}\text{Sn},p)^{133}\text{Sn}$ reaction. Also, in the $d(^{132}\text{Sn},p)^{133}\text{Sn}$ reaction, the profile of the recoil nuclei at the end of the magnet shows they will not be able to be separated from scattered beam particles. The profile shows at most a 5 mm divergence, and unstable beams at ATLAS generally have beam profiles of approximately that size.

QUARTZTOF: Developing a Simulation of a New Cerenkov Time of Flight Counter for Proton-Proton Interactions in the Large Hadron Collider

Kristina Yancey (TEXAS A&M UNIVERSITY, COLLEGE STATION, TX 77843), **Hans Wenzel** (FERMI NATIONAL ACCELERATOR LABORATORY, BATAVIA, IL 60510). The search for the Higgs Boson, one of the most popular topics in modern physics, will be at the forefront of objectives for the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) laboratory near Geneva, Switzerland. To detect forward protons that may have been involved in the creation of a Higgs Boson, the FP420 Research & Development Project is being developed to place detectors 420 meters downstream from two interaction points in the beam of the LHC. In order to accurately determine if a detected proton came from a specific interaction, timing resolution of about 10 picoseconds must be used in the FP420 detector, a problem that could be solved by QUARTZTOF, a new time of flight counter whose geometry is optimized to ensure that all Cerenkov photons produced when a relativistic proton (7 TeV at the LHC) passes through a cone-shaped Cerenkov radiator, arrive isochronously at a photodetector. In order to get approval for QUARTZTOF, simulations of the process must be created to show its precision. These simulations were created using Geant4, a framework that simulates processes as particles move through matter. Their data was then analyzed using ROOT, an object-oriented analysis program developed by CERN to investigate particle physics data. The geometry for the simulations was developed to match the real dimensions of the prototype with the exception of the cone's angle, which was set at half the angle of the Cerenkov radiation at a specific wavelength. When the simulation shot a proton directly along the axis of the cone, the timing resolution was an impressive 1.25 picoseconds; however, as the proton moved off the axis of the cone, the timing resolution became noticeably larger. This may pose a potential problem since in reality, the read-out detector can only register the timing of the photons, whereas the simulations showed how sensitive QUARTZTOF is to the position of the proton as it travels through the cone. The simulations highlighted the fact that the geometry is not as simple as it was thought to be, and more effort must be made to account for the variations produced as the proton moves away from the axis of cone.

Determining Spatial Extendedness of Gamma-ray Large Area Space Telescope Sources

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In order to identify the origin of photons detected by the Gamma-ray Large Area Space Telescope (GLAST), an effective method for classifying and parameterizing astrophysical objects as point sources or spatially extended sources is desired. GLAST software package Gtobssim is used to simulate the detector's interpretation of various types of gamma-ray emitters and sourcefit is used to reconstruct parameters for the sources using these simulated files. Fits were run using many different settings available in sourcefit to determine how to use the program most effectively, and sources of various sizes, fluxes and spectra were modeled to determine the parameter limits for this analysis. No compelling reason was found to change the default values of sourcefit's settings and fit quality was discovered to improve significantly with increasing flux and decreasing spectral index. Test Statistic (TS) value was seen to decrease rapidly as spectral index increased, suggesting that soft spectrum sources are more difficult to parameterize due to more of their photons being mistakenly characterized as background radiation. Future research should include testing in the presence of more realistic background radiation, as well as a more descriptive quantification of sourcefit's accuracy.

Science Policy

Biofuel Refinery Site Assessment in the Pacific Northwest

Ryan Butner (UNIVERSITY OF WASHINGTON, SEATTLE, WA 98195), **David Anderson** (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352). As the United States faces increasing concerns over the pricing and security of energy resources, biofuels have become increasingly appealing. The confluence of modern economics, concerns over carbon emissions, politics, and new refining methods now make bio-ethanol and biodiesel commercially viable energy alternatives to petroleum based fuels. What is not understood is the balance between biofuel demand and supply in the Pacific Northwest (Washington, Idaho, and Oregon). To answer this, the Biofuel Mandates and Mass Balance: Community-Level Socioeconomic and Land Use Impacts in the Pacific Northwest study will create a series of maps based on a range of employment and economic data sets to identify sites with ideal economic conditions for a biofuel refinery. The information used to generate these maps was primarily collected from the U.S. Department of Labor's Bureau of Labor Statistics online database. Specifically, the focus of data collection from this database was on agricultural production, average income, and unemployment rates for individual counties in the Pacific Northwest as indicators of overall economic health and potential receptiveness to new biofuel refineries. This data was combined in spreadsheets using Microsoft Excel for analysis and for future entry into a geographical information system (GIS). Like previous studies, this work will later be focused on the potential economic impacts from hypothetical refineries near rural communities using economic impact modeling software such as IMPLAN (IMpact analysis for PLANning). Unlike other studies, this project will produce visual guides in the form of maps to clearly represent the several subregions within the Pacific Northwest and determine the overall viability for a refinery in that area. Portions of this project will later be used to produce more case studies on the economic impact of biofuel refineries.

Writing Science News and Feature Stories for the Brookhaven National Laboratory Media & Communications Office

Kirsten Dorans (MCGILL UNIVERSITY, MONTREAL, QC H3A 2T5), **Kendra Snyder** (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973). Brookhaven National Laboratory's (BNL) Media & Communications (MedCom) Office provides information about research, events, policies and procedures at BNL for internal and external audiences with the goal of promoting BNL's international reputation as a world-leading multidisciplinary research center. As a MedCom intern, I worked alongside BNL staff writing science news and feature stories for different media outlets. I used a variety of resources to accomplish this including: interaction with the MedCom staff; interviews with BNL researchers, staff and other summer interns; past MedCom publications; online news and government resources; and Microsoft Word. Throughout the editing process, I often communicated with sources and MedCom editors until the writing was clear and concise. I wrote articles for The Bulletin (e.g., "Cicadas On Site"), a weekly newspaper for employees and users; stories for Brookhaven's website (e.g., "Meet Vicky Giese"); and I worked on news releases about BNL research. Throughout the summer, I helped the MedCom Office staff effectively provide up-to-date information about Brookhaven to employees, users and the public.

Science Writing Reflective Essay and Portfolio

Zoe Macintosh (SMITH COLLEGE, NORTHAMPTON, MA 01063), David Harris (SLAC NATIONAL ACCELERATOR LABORATORY, STANFORD, CA 94025).

The purpose of science writing is to communicate science to a general audience, a function important for keeping non-technical people informed in an increasingly technical world. The main goal of this project was to report on the research projects of the Science Undergraduate Laboratory Internship (SULI) student cohort at the SLAC National Accelerator Laboratory (SLAC) and prepare articles about their research which are accessible to non-scientists. The main goal of science writing is to convert raw information into text with a clear focus and story. Writing about science at SLAC gave experience in approaching complex subject matter and distilling its important elements into such text through a process that involves background research, interviewing, asking follow-up questions, writing to learn, writing drafts of the article itself, and integrating scientists' edits in the approval stage after the article is completed. In learning about science and the work that colleagues are doing, many lessons about science writing become apparent. Journalism differs from other forms of writing in that it is plain, direct, and concise. Gaining clarity about what one is going to write before one writes it significantly affects the quality of the writing and the ease of the experience. The interview can be a critical stage in the interview process, because it engages two levels of understanding in a dialectic inherently filled with story-resources. In order to bridge levels of understanding between a specialist and a non-specialist, it is important to retain a balance in technical immersion: too little research will make it difficult to identify what is interesting; too much will make it difficult to have the detachment necessary to produce a successful translation. To prepare stories on the work of other SULI students, various reference materials were needed. They included scientific papers and explanatory articles, but they primarily included notes from interviews with SLAC scientists and summer students. By the end of the program, I had created a set of articles about the research of SULI students, accessible to non-scientists who would have trouble reading technical papers. This was an experimental variant on the SULI internship program that helped add value to the research done by other SULI students, and also trained me further in the exploration of complex scientific topics and the communication of them to lay audiences.

* Information Mining for Transportation Security Needs

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Ammonium nitrate is readily available and widely used as a fertilizer. In its solid state, at a normal temperature and pressure, it is a stable chemical. However, when combined with other substances or factors, it can turn into a weapon for terrorist attacks. This project examined the use of public transportation as a potential means for evacuating special-needs populations, especially during this form of attack. Using data from multiple sources, including the National Transit Database of the Federal Transit Administration, this study first reviewed the transit system as a whole. In performing this review, we considered various aspects of the transit system, including the top 50 agencies with the most vehicles available at maximum service, the amount of gross revenue, and the number of unlinked passenger trips. For a more detailed analysis, the project then focused on the special-needs population of the Chicago-Naperville-Joliet (IL-IN-WI) Metropolitan Statistical Area (MSA). We examined data on this population (organized by age and income), including households without cars, possible shelter locations, and modes of transportation, using RailReady, a risk assessment system developed by the Center for Transportation Analysis. A small section of the MSA was then selected to assess the practicality of using the transit system to aid during an ammonium nitrate evacuation. Taking into account the loading, unloading, and travel time, we calculated that it would take approximately 2.5 to 4 hours to evacuate 12100 special-needs people in this area. Results of our study show that using public-transit vehicles could be beneficial in an emergency evacuation in the chosen section of Chicago.

Developing a Searchable Keyword Inventory for Standards-Based Management System (SBMS) Subject Areas

Nicole Puglin (EMERSON COLLEGE, BOSTON, MA 02116), Katherine Orta (BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973).

A keyword inventory was created for the Standards-Based Management System (SBMS) at Brookhaven National Laboratory (BNL) in order to make Subject Areas more easily searchable by staff. Subject Areas are documents accessible on the SBMS webpage that translate requirements into Laboratory-wide procedures for practical implementation by staff. The keyword inventory is a comprehensive list of key terms from each of the 145 SBMS Subject Areas (SAs). To

create the keyword inventory, each SA was first carefully reviewed and keywords were identified manually. Identified keywords were compiled using Microsoft Word. The SBMS Keyword Management web-tool was then used to manually transfer the keywords onto the SBMS webpage and link them to specific sections of the correlating SAs. The keyword inventory acts as a search engine so that a user can enter a search term and the result will be a direct link to all of the SAs that mention that term. The creation of the searchable keyword inventory is a small portion of a larger, ongoing effort to improve the SBMS website and increase its usability. In the future, the keyword inventory will allow Lessons Learned documents that report positive and negative operating experiences at BNL to link with related SAs on the basis of common keywords.

The Critical Role of the Mass Media in Public Understanding and Perception of Science

Caitlin Shenk (LEHIGH UNIVERSITY, BETHLEHEM, PA 18015), Mary T. Beckman (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352).

Scientific and technical matters are playing an increasingly critical role in many aspects of modern society. We now live in a world where the general public needs access to useful, convenient, and understandable scientific information for their day-to-day lives. People want to know: What is climate change, and what impact will it have on my life? Are products with nanoparticles safe to use, and do they possess any advantages over products without nanoparticles? Will alternative sources of energy really impact our dependence on foreign oil, and what changes will I need to make in my everyday life as a result? For the public to make decisions on science-based issues, they must first understand them. Science communication, as a discipline, aims to improve the distribution and comprehension of scientific information for the general public. Science writers serve as conduits among inventors, researchers, and the public. In recent years science communicators and scientists have made an enormous effort to improve the understanding of science and technology among the general public. In order to observe and experience the complex interplay between science and communication in the national laboratory setting, I interacted with communicators and engaged researchers at Pacific Northwest National Laboratory (PNNL) in Richland, Wash. Through these interactions, I developed a variety of communication tools, including press releases, tip sheets, news pitches, and media events. My experience at PNNL not only further developed my writing skills, but exposed me to new aspects of the communication process, including direct interaction with the mass media, and equipped me with the tools to communicate more effectively.

Initial Evaluation of the Science Teacher and Researcher (STAR) Program

Zack Valdez (ST. MARY'S UNIVERSITY, SAN ANTONIO, TX 78228), Dr. Susan Schultz (SLAC NATIONAL ACCELERATOR LABORATORY, STANFORD, CA 94025). The California State University (CSU) system strives to increase the development of high quality math and science teachers. To attract and retain K-12 educators with a better knowledge of subject matter and investigative skills, the Science Teacher and Researcher Program (STAR) program links scientific research experiences with teaching. Through private funding and with leadership from CSU, STAR provides science majors, interested in teaching, an eight week internship at a national lab. Participants engage in science research to better understand their dual roles as teachers and researchers in society. This segment of the evaluation study consists of analyzing application data, observing lab sites, and conducting interviews to determine ways the program can improve while measuring its success. Participants studied consisted of a group of 19 females and 11 males ranging in age from 20 to 57 years, with career levels from undergraduates to full-time teachers. Preliminary findings indicate that a majority of participants stated the program provided them with a wider scope of knowledge and deeper understanding of specific fields. Clarifying concepts and explaining real world applications to their students are examples of skills that participants noted as benefits from their research experience. Participants learned that scientists don't arrive at one right answer but rather use multiple paths during investigations. Identified areas for program improvement include better alignment between research projects and a participant's field of study and more communication between mentors and interns about the project. Program developers need to improve on making explicit connections between the nature of science and research experiences.

Waste Management

Inspection and Diagnostics of Nuclear Operations Waste Storage Facilities

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The Nuclear Operations Division (NOD) is responsible for several facilities on the Argonne National Laboratory site, most of which contain radioactive material, which entails the risk of contamination should the containment in any of the buildings be damaged or fall into disrepair. To maintain safety standards, the NOD must inspect all the facilities in its charge to ensure that nuclear material is properly contained, and that the containment equipment would function properly following such events as fires, high winds, and earthquakes. Inspection is aided by procedures that detail which areas of the facility must be inspected as well as what must be inspected in each area. NOD had a facility-specific combustible control procedure that applied to a single facility. This facility-specific procedure was modified to apply to all NOD hazard category nuclear facilities. Additionally, new natural phenomenon hazard inspection procedures were developed for each facility. Inspections of the facilities were then carried out to look for additional items that should be inspected. Reports compiled by engineering consultants and NOD Cognizant System Engineers (CSEs) were also reviewed to note specific items that should be inspected following various events. These included past Fire Hazard Analyses reports and Natural Phenomena Hazard Structural Evaluations. The procedures were then submitted for review and concurrence by the facility managers, fire protection engineers, and other subject matter experts. In addition, field walkdowns were made on the nitrogen supply to the Building 212 Alpha Gamma Hot Cell Facility to ensure that the tanks and piping providing an inert atmosphere to the facility were functioning correctly. The piping drawing for the nitrogen system was modified to reflect new valve positions previously unmarked. The efforts to improve nuclear facility inspection will ensure that facilities are inspected on a regular basis, that any repairs necessary are made, and that the various facilities the NOD inspects will be safe places in which to work.

Effect of Carbon Addition on Simulated Tank Waste Melting Rate

Carissa Humrickhouse (WHITWORTH UNIVERSITY, SPOKANE, WA 99251), Mike Schweiger (PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 99352).

Cleanup efforts at the Hanford Site in Washington State have been addressing 177 underground tanks which contain waste generated by weapons reprocessing following World War II and Cold War eras. A primary method of cleanup is vitrification, which combines nuclear waste with glass additives in a slurry, known as a feed. The energy required to melt a feed could be reduced if the melting rate was increased allowing cost and time to decrease. One method of increasing the melting rate is to add carbon sources to feeds that are high in nitrates. When carbon and nitrogen combine, an exothermic reaction occurs at 280 °C and the reaction heat accelerates the melting process. In this study, nitric acid was added to a High Alumina (HA) slurry until pH 1 was reached. The carbon sources used were cellulose and sucrose, each of which was added in a specific carbon to nitrogen ratio. Feeds were monitored while heated from room temperature to 1000 °C at 5 °C/min. Differential Thermal Analysis (DTA) and Thermogravimetric Analysis (TGA) techniques were used to compare feeds. Unlike the baseline, feeds that contained a carbon source initially expanded at 250 °C and then noticeably shrank. Using DTA and TGA, it was determined that an exothermic reaction occurred at 280 °C. This indicates the desired reaction was taking place in all the carbon-containing feeds. Continuing work includes scanning electron microscopy, X-ray diffraction analysis and characterization of heat transfer properties within feeds.

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