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# SCHEDULE OF EVENTS

## **8th Annual Student Research Day Schedule**

Roaden University Center, Multipurpose Room, 2nd Floor

### **April 10, 2013 (Wednesday)**

**12 – 4:00 p.m.** Poster Setup

### **April 11, 2013 (Thursday)**

Continental Breakfast

**8:00 – 9:30 a.m.** Judging  
Students will be available to discuss posters (if possible).

**10:00 - 11:15 a.m.** Poster Display for Review and Discussion  
Students will be available to discuss posters (if possible).

**11:15 a.m. – 12:00 p.m.** Awards Ceremony

**12:15 – 1:15 p.m.** Lunch

**12:00 – 2:00 p.m.** Poster Display Review and Discussion  
Students will be available to discuss posters (if possible).

**2:00 – 3:00 p.m.** Speaker Reception (Noble Cody Suite)  
(Students, Faculty and Staff are invited for light refreshments)  
Poster Pick-up

# CEREMONY

## **8th Annual Student Research Day Ceremony**

Roaden University Center

April 11, 2013

|   |  |
|---|--|
| <b>Welcome</b>  | Beverly McDonald-Robinson<br>Director Sponsored Programs and Creative Activities   |
| <b>Occasion</b>                                       | Mark Stephens<br>Interim Provost and Vice President, Academic Affairs  |
| <b>Introduction<br/>of Speaker</b>                    | Beverly McDonald-Robinson<br>Director Sponsored Programs and Creative Activities   |
| <b>Guest Speaker</b>                                  | Joe Matteo,<br>Division President, ProNova Solutions, LLC<br>Research & Development and Manufacturing  |
| <b>Recognition<br/>of Students</b>                    | Philip B. Oldham<br>President, Tennessee Technological University  |
| <b>Presentation<br/>of Awards</b>                     | Philip B. Oldham<br>President, Tennessee Technological University<br>Francis Otuonye<br>Associate Vice President, Tennessee Technological University |
| <b>Closing Remarks</b>                                | Beverly McDonald-Robinson<br>Director Sponsored Programs & Creative Activities   |
| <b>Speaker Reception<br/>&amp; Student Cross Talk</b> | 2:00 p.m. – 3:00 p.m.<br>Students, faculty and staff are invited to the Noble Cody Room<br>for light refreshments.                                   |

# ROUNDTABLE & LUNCHEON

## **8th Annual Student Research Day Speakers Roundtable and Luncheon**

Roarden University Center, Noble Cody Executive Suite, 2nd Floor

**April 11, 2013 (Thursday)**

**12:00 – 1:00 p.m.**

### **PROGRAM**

#### INVOCATION & INTRODUCTION OF SPEAKER

Beverly McDonald-Robinson, Ed.S.  
Director of Sponsored Programs and Creative Activities

### **PRESENTATION**

#### NATIONAL SCIENCE FOUNDATION

Kathleen V. McCloud, Ph.D.  
Director of Physics, Division of Mathematics and Physical Sciences

### **REMARKS**

Frances Otuonye, Ph.D.  
Associate Vice President of Research and Graduate Studies

### **BUFFET STYLE LUNCH**

(Move freely to the serving area)



April 11, 2013

Dear Student Investigators:

Congratulations on the outstanding display of investigative research you put forth by participating in Student Research Day. On behalf of the faculty, staff and administration of Tennessee Technological University, I commend you for your research and your commitment to work under the guidance of faculty research advisors. Your research brings honor and recognition to the University, the greater Cookeville community and the state of Tennessee.

Academic and practical research is an essential part of the university experience at every level, for both undergraduates and graduates, across all disciplines. It is your research and dedication that continue to position Tennessee Tech among the nation's best universities, as recognized regularly by The Princeton Review, *US News and World Report*, and others. The accolades bestowed upon Tennessee Tech are direct reflections of your commitment to scholarly activities and academic success. I appreciate your efforts, your investigative spirit, and your willingness to take your studies a step further by taking part in Student Research Day.

Sincerely,

A handwritten signature in black ink that reads "Philip B. Oldham". The signature is written in a cursive style with a long, sweeping underline.

Philip B. Oldham  
President



Dear Tennessee Tech Students:

Tennessee Technological University is strongly committed to active forms of learning and student research, at both the undergraduate and graduate levels. Student research has become a key component of our strategy to promote student success. Student Research Day not only enhances the acquisition of knowledge but also provides challenging opportunities to improve communication skills as the researcher transmits results through exhibits, presentations, and verbal interaction.

I am delighted to welcome everyone to Student Research Day 2013, a time for celebrating our commitment to active learning and a platform to showcase the work of dedicated students.

Sincerely,

Mark Stephens  
Provost and Vice President for Academic Affairs



#### WELCOME TO TENNESSEE TECH STUDENT RESEARCH DAY

Dear Students, Faculty and Community,

It is with great pleasure that we welcome you to the Student Research Day Poster Session. We take this opportunity to give you a glimpse of the research activities involving undergraduate and graduate students that take place in the different departments at Tennessee Technological University.

Students' participation in research is consistent with our commitment to the lifelong success of our students. Research stimulates active learning, increases critical thinking skills and effectively prepares our students for the workforce of the 21st century. It is through research that new knowledge is created and disseminated, and technology is developed and transferred to benefit society.

We express our appreciation to the students who have prepared and presented their posters, the faculty advisors who have mentored, guided and/or supervised the projects, and the Research Liaison Officers who have assisted us in planning and encouraging participation in the Student Research Day Poster Session. We are pleased with the opportunity provided by the Student Research Day for students to showcase their research endeavors. We hope that the projects will stimulate more interest in student research and other scholarly activities that enhance teaching and learning.

Thank you.

Francis Otuonye  
Associate Vice President  
Research and Graduate Studies



## MESSAGE FROM THE DIRECTOR OF SPONSORED PROGRAMS AND CREATIVE ACTIVITIES

Tennessee Technological University's 8th Annual Student Research Day provides an opportunity for the entire community to share research. It provides an additional platform for students and faculty to engage in scholarly dialogue and intellectual exchanges.

Students are encouraged to begin inquiry-based learning early in the matriculation. Sharing results of research closes the loop of the learning cycle and the benefits gained from the experience are numerous, including a sense of accomplishment and pride in one's work well done. A total of 140 student abstracts were submitted to the 8th Annual Student Research Publication, spanning across disciplines such as counseling and psychology, curriculum and instruction, human ecology, engineering, chemistry, biology, physics and earth sciences. We appreciate our faculty for the untiring leadership that emphasizes the discovery and advancement of knowledge through research. Student Research Day would not be possible without the support of our faculty, who are committed to quality research.

One other program highlight is the keynote presentation by Mr. Joseph Matteo, Division President of R&D and Manufacturing at ProNova Solutions in Knoxville, Tennessee. He is a recognized expert in nano-technology, with more than 20 patents and copyrights. We salute Mr. Matteo for his dedication to science and nurturing desire to develop new scientists. We thank him for taking the time to share sage words with our students, faculty, staff and guests.

It takes a super team to execute Student Research Day. On behalf of the Office of Research and Graduate Studies, I would like to express my gratitude to President Philip B. Oldham for his support and promotion of research and scholarly work, as well as being an active leader in the event. Also to the visionaries David and Sherri Nichols who believe in the power of research to the extent to establish an endowment to cultivate future student investigators, we sincerely appreciate your support. I also extend many thanks to the entire Tennessee Technological University staff for your services and cooperation, especially, Communications & Marketing, University Dining Services, and Facilities Services. We are indebted to our volunteers as judges; your time and effort ensures the quality and success of the competition.

Finally, I am most proud of Dr. Francis Otuonye and the Office of Research and Graduate Studies for being the champions of this event. I am sincerely grateful for the support of K'Cindra Cavin, Sandy Garrison, Jennifer Kirby, Mark Lynam, Kathy Reynolds, Sammie Sparks and Ellen Wolfe. Your time and talents are highly appreciated. I am proud to be a member of the team. Congratulations on a job well done.

On behalf of the Tennessee Technological University Family, I extend a heartfelt welcome to this day of discovery.

Beverly McDonald-Robinson, Ed.S.

# SPECIAL GUEST



**Joseph Matteo**  
**Division President of R&D and Manufacturing**  
**ProNova Solutions**

Joseph Matteo is the Division President of Knoxville-based ProNova Solutions, LLC R&D and Manufacturing and Vice President of Research and Development for the Provision Center for Proton Therapy. He has more than 20 years of technology experience with numerous patents and publications. Previously, he served as the Chief Technology Officer for Advion BioSciences when the company he founded, NanoTek LLC, was acquired by Advion. NanoTek was founded in October 2004 to pursue the development of micro and nano-scale technology for rapid production of radiolabeled imaging agents for use in positron emission tomography (PET). In its first 18 months, NanoTek successfully won five Small Business Innovation Research grants, filed multiple patent applications, developed several microfluidic products, secured development relationships with large pharmaceutical companies, medical device manufacturers, and leading research universities, and began marketing and selling commercial units.

Prior to starting NanoTek, Matteo spent 14 years with CTI Molecular Imaging. He served five years as the Cyclotron Systems Division Director. While at CTI, he managed a staff of 75, including R&D, manufacturing, production, installation, purchasing, service, and training, and led various quality-improvement and cost-reduction efforts. R&D efforts focused on development of three new automated chemistry instruments and a new cyclotron model, which is where he developed his interest in microfabrication and microchemistry. Before CTI, he led a small-business venture, Matteo Automation and Robotics, and found success developing anthropomorphic technology for NASA and for other prosthetic applications. He also spent six years in the military robotics field at Lockheed Martin and at the National Institute of Science and Technology.

Matteo is a mechanical engineer with a master's degree in controls and dynamics from the University of Maryland and a bachelor's degree from Drexel University.

# SPECIAL APPRECIATION & ACKNOWLEDGEMENTS

## SPECIAL APPRECIATION AND ACKNOWLEDGEMENTS

### Judges for 2013

|                          |  |
|--------------------------|--|
| Adams, Jeffrey           | Appalachian Center for Crafts          |
| Anderson, Adam           | Electrical & Computer Engineering      |
| Anderson, Melinda        | Human Ecology                          |
| Beck, David              | Biology                                |
| Callender, Andrew        | Chemistry                              |
| Carrick, Jessie          | Chemistry                              |
| Clark, Michael           | Honors Program                         |
| Coonce, Janet            | Chemistry                              |
| Crook, Amanda            | Chemistry                              |
| Cupp, Jan                | Counseling & Psychology                |
| Datta, Tania             | Civil & Environmental Engineering      |
| Demus, Nick              | Electrical Engineering                 |
| Eberle, William          | Computer Science                       |
| Elkeelany, Omar          | Electrical & Computer Engineering      |
| Elsawy, Ahmed            | Manufacturing & Engineering Technology |
| Ennis, Theresa           | Academic Affairs                       |
| Fidan, ismail            | Manufacturing & Engineering Technology |
| Fleming, Barbara         | Biology                                |
| Guo, Terry (Nan)         | Center for Manufacturing Research      |
| Han, Sang Moo            | Mechanical Engineering                 |
| Hart, Evan               | Earth Sciences                         |
| Hayslette, Steven        | Biology                                |
| Kalyanapu, Alfred        | Civil & Environmental Engineering      |
| Kamal, Ahmed             | Manufacturing & Engineering Technology |
| Kidd, Mary               | Physics                                |
| Knox, Larry              | Earth Sciences                         |
| Leimer, H. Wayne         | Earth Sciences                         |
| Lisic, Ed                | Chemistry                              |
| Nash, Jerry              | Education                              |
| Owens, Robert            | Minority Affairs                       |
| Porten, Michael          | Finance & Accounting                   |
| Rice, Cynthia            | Chemical Engineering                   |
| Rice, Jeffery            | Chemical Engineering                   |
| Sanders, Robby           | Chemical Engineering                   |
| Smith, David             | Mathematics                            |
| Stein, Barry             | Counseling and Psychology              |
| Stretz, Holly            | Chemical Engineering                   |
| Terneus, Sandra          | Counseling and Psychology              |
| Trent, Kristen Pennycuff | Curriculum & Instruction               |
| Whiteaker, Janet         | Education                              |
| Wilcox, Zachary          | Counseling and Psychology              |
| Work, Dale               | Chemistry                              |
| Zhang, Hong              | Chemistry                              |

### TTU Departments & Staff

#### Communications & Marketing

|                |  |
|----------------|--|
| Karen Lykins,  | Associate Vice President<br>for Communications & Marketing |
| Queena Jones   | Director of News & Communication                           |
| Lori Shull     | Writer, News & Communication                               |
| Dewayne Wright | Director of Creative Services                              |
| Lorie Worley   | Graphic Arts Technician, Creative Services                 |

#### Dining Services & Catering

|              |                   |
|--------------|-------------------|
| Victor Kline | Catering Director |
|--------------|-------------------|

#### Information Technology Services

|              |         |
|--------------|---------|
| Elaine Wells | Analyst |
|--------------|---------|

#### Office of Academic Affairs

|               |                          |
|---------------|--------------------------|
| Theresa Ennis | Director of Assessment   |
| Carol Holley  | Assistant to the Provost |
| Sue Ann Smith | Administrative Assistant |

#### Office of the President

|              |                            |
|--------------|----------------------------|
| Terri Taylor | Assistant to the President |
|--------------|----------------------------|

#### Student Services

|             |                          |
|-------------|--------------------------|
| Susan Henry | Administrative Associate |
|-------------|--------------------------|

## HUMAN ECOLOGY UNDERGRADUATE STUDENTS

### INVEST IN NUTRITION EDUCATION FOR COLLEGIATE ATHLETES

Elizabeth Miller, Dr. Cathy Cunningham,  
and Dr. Bruce Greene  
Faculty Research Advisor: Dr. Cathy Cunningham

The purpose of this research was to determine the ability of nutrition education programs to positively influence collegiate athletes' perceptions about the importance of diet quality and to improve diet behavior. Distance runners (n=22) from a mid-size Southeastern university were tested for self-efficacy and behavior using a qualitative survey and 3-day diet recall (ASA24 analysis) before and after a 9-week nutrition education program. The education series consisted of various nutrition topics for endurance athletes, such as nutrient timing for optimal performance, hydration, healthy snacking, and travel nutrition. Different teaching methods, including lectures, email newsletters, cooking demonstrations, and interactive activities were incorporated to facilitate learning. ANOVA methods were used to determine significant changes in self-efficacy and dietary intake. Athletes' personal assessment of diet adequacy was not well founded, but their willingness to change improved. Both the females and males consumed too little carbohydrate and too much fat before and after education. Whole grain intake increased for male athletes but not females. Heightened awareness of food choices seemed to be the reason athletes consumed less food, however the nutrient density improved for some key nutrients (Vitamins C, D, Saturated fat for both females and males and Total Fat and Calcium for males). Finding the athletes were willing to make better food choices, as well as acknowledge that nutrition can affect performance was a positive result. The researchers recommend an investment in nutrition education for all collegiate athletes. The TTU Undergraduate Research and Creative Activity Program provided funding for the project.

### EFFECTS OF THREE MILK FAT PERCENTAGES IN FROZEN GREEK YOGURT

Elizabeth Miller and Tori Holcomb  
Faculty Research Advisor: Dr. Cathy Cunningham

The purpose of this experiment was to determine the effects that 0%, 2%, and 10% milk fat have on objective (consistency, thawing stability, and pH) and sensory (texture, flavor, and overall acceptability) attributes, while looking at nutritive and cost effectiveness values as well. The yogurt samples were scored subjectively for texture, flavor, and overall acceptability. The whole milk yogurt had the highest

overall rating coming in second in the texture category and first in the flavor category. The yogurt samples were tested objectively for nutritive value, cost, consistency, pH, freeze time and thawing stability. In the pH testing, there was a consistent trend amongst the samples showing that the higher the milk fat percentage the higher the pH levels, which was consistent with research collected. In nutritive value analysis, the 2% and 0% yogurts had almost triple the amount of protein than that of the whole yogurt.

### EFFECTIVENESS OF SELECTED STAIN REMOVAL PRODUCTS ON UPHOLSTERY FABRIC

Ashley Pitts and Bethany Seals  
Faculty Research Advisor: Dr. Lizabeth Self Mullens

The purpose of this study is to determine if commercially-prepared products provide better stain removal outcomes than home-remedy products on common tannin stains on upholstery fabric. The fiber content of the fabric under investigation is 81% cotton and 19% rayon. The hypotheses included a) commercially-prepared products will produce better stain removal outcomes than the home-remedy products, and b) the distilled water/vinegar home remedy solution will provide a better stain removal outcome than 7-Up® home remedy product.

The independent variable is the cleaning products including Resolve® Multi-Fabric Upholstery Cleaner, a 50% vinegar/50% water solution, and 7-Up®. The three stains are common tannin stains including coffee, tomato juice, and wine. The dependent variable in the study is the stain removal outcome of the three removal methods. AATCC stain removal test methods and a locally-developed test method were used to determine stain removal outcomes. Stain removal outcomes varied with the type of stain and the type of stain removal product.

### OPTIMAL TEMPERATURE FOR DYEING WOOL WITH KOOL-AID®

Caitlin Roach and Jaclyn Hall  
Faculty Research Advisor: Dr. Lizabeth Self Mullens

The purpose of this study is to determine the optimal dye bath temperature for dyeing 100% wool yarn with cherry Kool-Aid®. The hypothesis is that there will be no difference in dye uptake with dye bath temperatures of 200°F, 225°F, and 250°F. The independent variable is dye bath temperature. The dependent variable is dye uptake. Dye uptake was measured using the AATCC Grey Scale for Staining. The dye bath temperature of 200°F resulted in a greater dye uptake than either of the higher dye bath temperatures.

## BIOLOGY UNDERGRADUATE STUDENTS

### CONTROL OF NITROGENOUS WASTE LEVELS IN SMALL TANK FISH AQUACULTURE

Jarrold Boles, Dr. Upul Deepthike, and Dr. Brad Cook  
Faculty Research Advisors: Dr. Upul Deepthike and  
Dr. Brad Cook  
Collaborator: Dr. Jeffrey O. Boles

Reports published recently indicate that nanoparticles incorporated into various man-made products are being released into the aquatic environment, primarily through wastewater treatment plants. Exposures to nanoparticles have been shown to lead to numerous biological and toxicological effects in aquatic organisms. A differential expression proteomic strategy could be selected to examine the effects of nanoparticles on living organisms; however, aquaria culturing techniques would have to be designed to not negatively affect test organism's health during the exposure period. This is especially challenging when non-model species are used as the test organism because of the lack of knowledge on their culturing conditions in the laboratory. The test organism used in this research is *Ictalurus punctatus* (Channel catfish) a both commercially important species as well as one taken by private anglers. The effect of nanoparticles on *Ictalurus punctatus* health is unknown at this time. Aquaria were designed to house catfish for a 30-day exposure to gold citrate-covered nanoparticles. A method for the determination of ammonia levels was developed to monitor levels of  $\text{NH}_3/\text{NH}_4^+$  while variables such as frequency of water changes and ionic strength levels were adjusted. The results of the study will be presented.

### LATE WINTER FOOD HABITS OF WHITE-TAILED DEER IN EAST TENNESSEE

Justin Hamby, Brian Thompson, and Joe Ellis  
Faculty Research Advisor: Mr. Keith Gibbs

The popularity of hunting white-tailed deer (*Odocoileus virginianus*) has increased across the entire country, especially in the southeast. Therefore, management of this game species is very important, not only for the hunting community, but for all natural resource enthusiasts. For management to be effective, data has to be collected to determine management successes. This study was conducted on the white-tailed deer's food habits in late winter in Rhea County, TN located in the southeastern part of the state. To determine food habits, trail cameras were placed above whole kernel corn plots and whole kernel corn plots with a persimmon gel scent added. The positions of

the plots were relocated weekly for five weeks resulting in a total of 10 different sites. Data collected included the time of day deer visited the plots, amount of time it took deer to find the corn, and amount of corn consumed at each site. After the data are collected, the purpose is to compare the two different sites to see what differences there are in the 3 categories. This research is ongoing. Results will soon be completed. Based on previous research, we expect there will not be that much of a difference between the two.

### ANTI-MICROBIAL SOAP VS. ALCOHOL-BASED HAND SANITIZER

Blake Huddleston, Amanda Randolph, and Clint Pitts  
Faculty Research Advisor: Mr. Keith Gibbs

In recent years, there has been an increasing amount of hand sanitizer made available in everyday life. Schools, healthcare facilities, and the workplace have implemented these products in order to increase hand hygiene and reduce the spread of illnesses. This research determines the effectiveness of antimicrobial soap versus alcohol-based hand sanitizer. A group of 10 volunteers were used to determine which product was more efficient. These individuals washed their hands using the APIC hand washing technique. Of the ten individuals, five of them washed their hands with anti-microbial soap and the other five washed their hands with an alcohol-based hand sanitizer. This research is still ongoing and results are to be completed soon. However, from previous research, it is expected that alcohol-based hand sanitizer is more effective at killing bacteria that are present. A t-test will be done in order to determine the statistical difference between the two products used.

### CELL PHONES: A RESERVOIR FOR STAPHYLOCOCCUS AUREUS

Adrienne Kane, Rusty Arwood, and Ashley Nash  
Faculty Research Advisor: Dr. David Beck

Objective: To determine if the cell phones of students at Tennessee Technological University are significant reservoirs for *Staphylococcus aureus*.

Methods and Results: Staphylococci were cultured from 121 cell phones of students. Polymerase Chain Reaction (PCR) analysis revealed 43 of the cellular phones (35.5%,  $n=121$ ) were contaminated with *S. aureus*, and 5 of the phones (4.1%,  $n=121$ ) carried multiple isolates of *S. aureus*. Of the 48 *S. aureus* positive isolates found using PCR, further testing will be conducted to determine minimal inhibitory concentration (MIC) susceptibility in response to various antimicrobial agents.

Conclusion: *S. aureus* was identified on 35.5% of student cell phones.

Significance and Impact of the Study: The study demonstrated the significant frequency of *S. aureus* contamination of cellular devices in the university setting.

### AFFECTS OF OIL POLLUTION ON NATIVE CRAYFISH IN THE PRESENCE OF DAWN®

Nathan Karch and Jordan Cross  
Faculty Research Advisor: Dr. Daniel Combs

We are concerned about the health risks that oil pollution poses toward native crayfish populations. The effects of oil pollution on vertebrates have received a great deal of scientific attention, but little focus has ever been given to invertebrates. We wanted to determine how crayfish are affected by oil pollution in aquatic ecosystems with the presence of DAWN® dishwashing detergent acting as a surfactant. DAWN® has been used over the last 30 years as a degreasing agent to help cleanse wildlife affected by oil spills, consisting mainly of vertebrates. We set out to investigate if DAWN's® degreasing and cleansing properties provide the same benefits to invertebrates. Crayfish were caught in local streams using traditional baited trapping methods. The crayfish were placed in artificially simulated environments using three, ten gallon freshwater aquariums at five individuals per tank. In our experimental study, one tank was exposed to used motor oil and the other exposed to used motor oil in the presence of DAWN® dishwashing detergent. We used high concentrations of oil in each experimental tank to imitate a devastating oil spill. In each experimental group, we ran a series using five trials. Each trial will be conducted over a period of three days. This research is ongoing and results will be completed soon. However, based on previous research, we expect higher crayfish mortality after prolonged exposure to the high concentrations of oil in the absence of DAWN® than in the presence of DAWN®.

### EFFICACY OF MOUTHWASH WITH AND WITHOUT ALCOHOL: AN IN VITRO STUDY

Kenji Maeda  
Faculty Research Advisor: Mr. Keith Gibbs

The importance of plaque inhibition has long been documented and proven to be essential in proper dental hygiene. Several factors play a role in the decomposition of plaque ranging from mechanical to chemical elements. Since the introduction of chemical mouthwash use to aid in plaque prevention, various forms have been created in hope to obtain a solution that has the greatest effect on

plaque as well as the least amount of alternative effects on the user. The two mouthwashes studied came from the same manufacturer (Listerine), one containing an alcohol content of 21.6% and the other including essential oils claiming to possess the same antibacterial, anti-plaque effect as the alcohol-containing product. The presumption that these two mouthwashes are equivalent in the suppression of bacterial accumulation was tested. The study design involved the inoculation of bacterial samples in mouthwash solution for a 30 second exposure time, after which a sample was taken and allowed to culture. Observation of each sample under a microscope was taken and statistical analyses of the mean total bacterial count were tested between the two mouthwashes. Research is currently in process. Results will be completed soon. Based on previous related studies, I expect a statistical difference between the two products, with better plaque restraint in the mouthwash containing alcohol. Further studies should be taken to assess how time and frequency of use factor into the overall growth of the plaque.

### COMPUTATIONAL STUDY OF ACETYLTHIAZOLE THIOSEMICARBAZONE CONFORMATIONS

Mallory Miles and Dr. Scott Northrup  
Faculty Research Advisor: Dr. Scott Northrup

Computational modeling procedures within Hyperchem software were used to produce sixteen conformations of thiosemicarbazone acetylthiazole (ATZ-TSC). Beginning with a planar model of ATZTSC containing four trans bonds, bond torsions were adjusted to create conformers with varying combinations of cis-and trans-bonds. Preliminary structures were then subjected to semi-empirical AM1 (Austin Model 1) quantum calculations, which produced more accurate, geometry-optimized conformers of the original molecules. Relative energies, degree of planarity, and existence of internal hydrogen bonding were compared for each conformer. Conformers obtained from AM1 calculations were subjected to higher level quantum mechanics (following the ab initio Hartree-Fock method) in order to produce still more accurate models of the conformers of ATZ-TSC. At the end of these calculations, conformer energies were extracted and used to produce a table of relative energies. Some discrepancies in the relative energies of AM1 and ab initio conformers were found to exist. The ab initio relative energies were taken to be more accurate, and variations in the AM1 conformers were taken as indication of the necessity of the higher level quantum mechanics. Finally, a catalogue of model images was prepared depicting the different conformers. Comparison of the conformer images with their relative energies revealed a positive correlation between the conformers of lowest relative energies and those containing internal hydrogen bonds. ATZ-TSC

conformers determined to exist at lowest energies are believed to be those which would occur in greatest natural abundance, distinguishing these structures as candidates for focus in subsequent studies involving intermolecular interactions with ATZ-TSC.

## TASTE PREFERENCE OF LOW-FAT VS. REGULAR FAT FOODS

Brenden Phillips  
Faculty Research Advisor: Mr. Keith Gibbs

Many low fat foods claim to provide the same taste as its regular fat counterparts. However, when fat is taken out of regular fat foods, something else is added as a fat supplement. These additives are usually supplements such as salts, sugars, and artificial flavorings. My experiment is designed to test if low fat foods taste the same as the regular fat foods. My experiment consists of 5 trials with 10 people in each trial group. I used two dry products (chips and bread) and two dairy based products (milk and yogurt) in the experiment. I used the same brand for each low-fat and regular fat item. Subjects conducted a blind taste test to determine taste preference for each food item. Research is ongoing, but results from three trials have displayed that women were more likely to pick low fat dry foods at 15% more of the time compared to their male counterparts. However, overall results show greater preference for regular fat dry foods, yet there was no distinct preference for either type of dairy product. Completed results should verify observed trends.

## BACTERIAL REGROWTH OF ORAL MICROBES USING ALCOHOL AND ALCOHOL-FREE MOUTHWASH

Johanna Trevino and Jenna Raulston  
Faculty Research Advisor: Mr. Keith Gibbs

Microbes, naturally found in the normal oral environment of humans, form biofilms on teeth. Although most oral microbes are harmless and often beneficial to humans, many are naturally pathogenic and some have become resistant to antiseptic treatment. These types of bacteria can lead to serious dental diseases such as gingivitis, periodontitis and plaque formation on the teeth. The purpose of this experiment is to test the effectiveness of alcoholic and nonalcoholic mouthwash on the bacteria present in the oral cavity. Crest Pro Life® alcohol free and Cool Mint Listerine® Antiseptic mouthwashes were used for this experiment. We were the subjects of the experiment and avoided using dental hygiene products 24 hours prior to the experiment. Before treatment, we collected oral swabs to establish a baseline for amount of oral bacteria present. We then rinsed

with mouthwash and collected oral swabs every fifteen minutes for one hour. This procedure was repeated during 5 trials for each subject. The bacterial samples were then allowed to incubate in a nutrient rich agar for 8 days. After which, bacterial growth was measured. This research is ongoing and results will be completed soon. However, based on previous research, we expect the alcoholic mouthwash to inhibit bacterial growth for a longer period. Mouthwash is an essential part of dental hygiene, but further studies should evaluate the effectiveness and safety of using alcoholic versus nonalcoholic mouthwash.

## BORRELIA AND EHRLICHIA IN RIPHICEPHALUS SANGUINEUS COLLECTED FROM DOGS IN SOUTH TEXAS

Rosa Vasquez  
Faculty Research Advisor: Dr. David Beck

Laredo, Texas veterinarians have recently reported Lyme disease, the most common tick-borne disease in the Northern United States, to be present in dogs. Rhipicephalus sanguineus (brown dog tick) is endemic throughout the world wherever dogs are present. These ticks were collected and their DNA was purified using the EZNA Mollusk DNA isolation kit. Samples were screened to determine the prevalence of Borrelia species (vectors of Lyme disease and STARI – disease that resembles Lyme disease – are included), Rickettsia and Ehrlichia species (vectors of Rocky Mountain Spotted Fever and Ehrlichiosis respectively). These species can also be infectious for humans.

Polymerase chain reaction was used to amplify DNA samples. We are in the process of screening positive samples and confirm results by DNA sequence analysis. Borrelia lonestari in 17.7% (n=19/113) samples, other Borrelia species in 9.7% (n=11/113), and Ehrlichia in 12.4% (n=14/113) were detected. This report expands the distribution of STARI into South Texas. Research continues to determine if the species causing Lyme disease is truly present. This data may help develop a better protocol of treatment for dogs and will increase awareness of possible expansion of tick-borne diseases.

## A POPULATION STUDY OF THE EFFECT DESEXING CANINES HAS ON LIFESPAN

Michele Claire and Billy York  
Faculty Research Advisor: Mr. Keith Gibbs

Desexing, also known as neutering and spaying, is the surgical removal of an ovary or testis. In the United States veterinarians, along with animal group activists, encourage canine owners to desex their canines so their pet has a

longer lifespan. As spaying and neutering has increased since the 1970's the rise of obesity, endocrine disorders such as diabetes, seizure disorders and cancer in canines has been documented. When compared to Europe, where it is illegal to desex any animal, canines in the United States suffer from far different, more aggressive, cancers. Desexing a canine, in shelters, is performed at four to six weeks of age. We want to see how desexing affects their lifespans, how the procedure affects hormones, and which diseases and the seriousness of the diseases the two groups get to see if they are affected differently.

## CHEMISTRY GRADUATE STUDENTS

### ANALYSIS OF DIFFERENTIALLY EXPRESSED PROTEINS IN ESCHERICHIA COLI WHEN EXPOSED TO L-TELLUROMETHIONINE

Kathleen M. Broderick, Dr. Upul Deepthike,  
and Dr. Jeffrey O. Boles  
Faculty Research Advisor: Dr. Jeffrey O. Boles

Analysis of the three-dimensional structure of a protein using x-ray crystallography can be improved by the incorporation of unnatural amino acids. Most naturally occurring atoms do not have sufficient mass to diffract electrons, thus, heavy atom derivatives of target proteins are required. An unnatural amino acid, L-Telluromethionine (TeMet), which provides the necessary scattering power, has cytotoxic effects which reduce cell growth and uptake. A proteomic analysis of telluromethionyl *Escherichia coli* was carried out using the methionine auxotroph *E. coli* DL41 (DE3) (pCock) expression system. Both telluromethionyl and methionyl exposed cultures, before and after induction, were analyzed with the objective of identifying differentially expressed proteins. Analysis was carried out using 2D gel electrophoresis with isoelectric focusing as the first dimension and SDS polyacrylamide gel electrophoresis as the second.

Tryptic digestion and peptide fragment analysis using Nano-ESI/qTOF/MS/MS followed to allow peptide mass fingerprinting of differentially expressed proteins. Cell cultures were grown under typical conditions of recombinant protein expression with dihydrofolate reductase serving as the model recombinant protein. Insight into the biological roles of differentially expressed proteins could be used to improve methods of the TeMet bioincorporation. A more thorough understanding of the toxic effects of TeMet will provide information needed for the design of a novel growth media and/or required metabolic engineering necessary for improved x-ray crystallographic techniques.

### ANTI-PROLIFERATIVE PROPERTIES OF BENZOYLPYRIDINE THIOSEMICARBAZONE LIGANDS AND THEIR COPPER COMPLEXES

Jennifer D. Conner and Kathleen Mansour  
Faculty Research Advisor: Dr. Edward C. Lisic

Our research is centered on the anti-proliferative properties of benzoylpyridine thiosemicarbazone ligands and their accompanying  $\text{Cu}^{2+}$  and  $\text{Pd}^{2+}$  metal coordination complexes. The steps of our study included synthesizing several different forms of this ligand, saving some for future studies, and using some as reactors with metal ions. After obtaining the metal complexes, we then put all of our compounds through a series of bacteria studies, using the MIC (minimum inhibitory concentration) methods to test their activity.

### THERMAL STABILITY EVALUATION OF THE NEW GUANIDINE SUPPRESSOR FOR THE NG-CSSX

Talon G. Hill  
Faculty Research Advisors: Dr. Dale Ensor  
and Dr. Andrew Callender  
Collaborators: Dr. Laetitia Delmau (Oak Ridge National  
Laboratory) and Dr. Bruce Moyer (Oak Ridge National  
Laboratory)

The NG-CSSX employs a new more lipophilic guanidine to enhance the stripping of cesium from the solvent. The thermal degradation of this new guanidine was studied over time to evaluate its stability. The NG-CSSX solvent prepared with N, N', N''-tris(3,7-dimethyloctyl)guanidine (TiDG) was contacted and the performance tested with salt-waste stimulant SRS-15 over a period of three months at above-normal operating temperatures (35-37°C). An extraction, scrub, and strip (ESS) procedure was carried out at 25°C which included an initial extraction of cesium from SRS-15, two scrubs of the solvent system with 25mM NaOH to replace nitrate with hydroxide and remove potassium, and three strips using 10mM  $\text{H}_3\text{BO}_3$  to titrate the hydroxide and remove cesium from the solvent. The stability of the guanidine was critical to the stripping process as it suppresses the effects of competition anions that cannot be removed by the strip solution. The results show that prolong exposure to above normal temperature degrades the guanidine and reduces the efficiency of stripping cesium from the solvent.

## MICROFLUIDIC PAPER-BASED DEVICES FOR TITRATION OF CADMIUM

Shengxi Jin

Faculty Research Advisor: Dr. Andrew Callender

This poster presents a new device to measure the cadmium in water samples by titration with colorimetric reagents. A printer deposits wax patterns on filter paper which define channels with constant width. A water sample wicks through the channels (and reagents) by capillary action. We have used several different thiosemicarbazone ligands (TSC) for detecting cadmium (II). The ligand solution is spread over an area of the paper (10 to 100 mm<sup>2</sup>) and dried. The ligand should show only a faint color without cadmium, and an intense color when cadmium is bound. We quantify cadmium concentration by titration, instead of just color intensity: The reagent is present in the device at a uniform concentration (molecules of ligand per unit area). When the analyte is present, it reacts and is removed from solution, changing the paper color in that spot. By measuring the area of the paper that has changed color, we can calculate the amount of ligand reacted, and therefore the amount of metal present in the sample. This area measurement is very easy, needing only a ruler to measure the length of the colored bar! The advantages of PBDs are convenience, portability and low materials cost. They are easy to operate and require no electricity. This makes them more suitable for analysis of drinking water in developing countries and other areas with limited resources.

## DETERMINATION OF SOURCES OF ORGANIC POLLUTION IN NATURAL WATERS BY LCMS

Sreedharan Lakshmi Narayanan

Faculty Research Advisor: Dr. John Harwood

High levels of organic pollution cause low dissolved oxygen concentrations in water by "fueling" high bacteria concentrations, stressing both fish and the stream insect population upon which fish feed. Apart from lowered oxygen concentration, identification of human source pollution leads to secondary concerns: a) the possible presence of toxic trace pollution, harmful to aquatic life and potentially to human health, b) the possible presence of "emerging contaminants", pharmaceuticals and personal care products, which are found to be harmful to aquatic life and potentially to human health, and c) the possible presence of human source bacteria and viruses is indicated by the presence of human source organic pollution. Organic matter from different sources may be expected to have different impacts on aquatic organisms, and understanding those differing impacts will require accurate identification of the source of organic matter. Monitoring

changes in source loadings of organic matter will also be very important in understanding of the impacts of climate change on stream ecology. The bile acids and sterols in animal excreta are considered to be indicators of agricultural animal production waste contamination. These components are found to be stable in water but are present as non-polar substances that are associated with sediment and suspended particulate materials. They are never found dissolved in rivers or streams. Developing an LC-MS/MS method to analyze bile acids and fecal sterols would be a major step forward in using these biomarkers in environmental analysis.

## CHIRAL SEPARATION OF CLANDESTINE ATS AND CATHINONE DERIVATIVES BY HPLC-MS/MS

Sravan Mansani

Faculty Research Advisor: Dr. Jeffrey O. Boles

The abuse of illicit drugs, such as amphetamine type stimulants and cathinone derivatives, has been a major cause of concern in the State of Tennessee, as well as throughout the world. Including chirality in the chemical fingerprint database can potentially allow for rapid determination of starting materials used for synthesis, but it can in theory also provide identity to a specific cook. The objective of this research is to incorporate needed enantiomeric resolution data of seized clandestine drugs in the regional chemical fingerprint database to further differentiate between clandestine chemists. The separation of enantiomers is carried out by means of chiral chromatography coupled with tandem mass spectrometry. The stationary phase is a chiral CBH column, where the chiral selector is a protein cellobiohydrolase. The liquid chromatography method for separation of enantiomers using stock standards has been optimized. The clandestine samples are extracted and analyzed using optimized HPLC method.

## ARTIFICIAL SWEETENERS AS CHEMICAL MARKERS OF ORGANIC WATER POLLUTION

Sushma Meka and Dr. John Harwood

Faculty Research Advisor: Dr. John Harwood

The project focuses on determining if artificial sweeteners can serve as markers of the water contamination. To be an ideal marker, a compound should be source specific, should not react in waters but should be present in detectable quantities, and should be able to give good reproducibility in analysis (1). Sucralose and Acesulfame-K are two commonly used artificial sweeteners. These compounds are very water soluble, are not metabolized in the body, and are not removed in waste water treatment (2). They are being

studied as markers of waste water impacts in fresh waters in both the United States and in Europe (1 -4).

We are developing means of rapidly analyzing for Sucralose and Acesulfame-K in water samples by liquid chromatography-mass spectrometry (LC/MS). Analysis requires that the samples be pre-concentrated. We are comparing efficiency of preconcentration by different solid phase extraction (SPE) media. Liquid chromatography of these compounds is challenging due to their high polarity. We have compared retention of the compounds on a number of chromatographic stationary phases. Mass spectral sensitivity for sucralose is low with the electrospray interface, and we have tested post-column addition of TRIS buffer to enhance this sensitivity (4). We will present the detailed results of our method development for analysis of sweeteners in natural waters by LC/MS.

#### References:

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### THEORETICAL INVESTIGATION OF P-BENZOQUINONE REACTIVITY WITH N-CONTAINING NUCLEOPHILES

Lasantha Rathnayake  
Faculty Research Advisors: Dr. Scott Northrup  
and Dr. Titus V. Albu

Quinones are a class of organic compounds with a six membered unsaturated cycle with two carbonyl groups, either adjacent to each other or separated by a vinyl group. Because of their biological and industrial importance, quinones have been studied for decades and are still subject to recent studies. The purpose of this study is to investigate the reactions between quinones (p-benzoquinone, chlorop-benzoquinone and methyl-p-benzoquinone) and N-containing nucleophiles; (ammonia, methylamine and ethylamine). All the theoretical calculations were performed using Hybrid Density Functional Theory (HDFT) of mPW1B95-44 in conjunction with 6-31+G (d, p) basis set. Detailed conformational analysis was carried out for some of the reaction products and partial conformational analysis were carried out for the remainder. For all the considered reaction paths, most of the saddle points were located and optimized. Possible reactant complexes were identified to get better understanding of overall reactions. Two, four,

sixteen, sixteen and six saddle points respectively were optimized for the following reactions: p-benzoquinone with ammonia, p-benzoquinone with methylamine, chloro-p-benzoquinone with methyl amine, methyl-p-benzoquinone with methylamine and pbenzoquinone with ethylamine. In addition, collectively about twenty five product conformations were optimized for the above reactions. According to this obtained information, minimum reaction paths were identified for the investigated reactions. Analysis of the data is ongoing.

### SYNTHESIS AND BACTERIAL INHIBITION STUDIES OF ACETYL-PYRAZINETHIOSEMICARBAZONES

Carrie Thompson, Alexandra Arriaga, and Kathleen Mansour  
Faculty Research Advisor: Dr. Edward C. Lisic

New heterocyclic thiosemicarbazone derivatives of 2-acetyl pyrazine, 2-acetyl-3-methylpyrazine, and 2acetyl-3-ethylpyrazine have been synthesized, correlated, and characterized by <sup>1</sup>HNMR. These substances were used as tridentate ligands with Pd<sup>2+</sup> and Cu<sup>+</sup> to form metal complexes which were screened for bacterial inhibition. They were tested for antimicrobial activity by determining the minimum inhibitory concentrations against four bacteria (*Bacillus subtilis*, *Staphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa*), two yeast (*Candida albicans* and *Saccharomyces cerevisiae*), and one mold (*Aspergillus niger*). Entries made in previous literature pertaining to thiosemicarbazones indicate significant applications in biological and biomedical science.

### MUTATIONAL STUDIES ON THE CATALYTIC CORE OF HUMAN DNA POLYMERASE ETA

Adali Valdez  
Faculty Research Advisors: Dr. Xiaohua Jiang  
and Dr. Jeffrey O. Boles

The human DNA polymerase  $\eta$  (hPol $\eta$ ) specializes in bypassing UV-induced cyclobutane pyrimidine dimers formed from adjacent thymine bases by pairing the corresponding adenines during a process known as translesion synthesis. Patients with the variant form of Xeroderma Pigmentosum have a deficiency in hPol $\eta$ , are very sensitive to sunlight, and develop skin cancer in their early ages. Research shows that mutations in the hPol $\eta$  of XPV patients are directly linked to skin cancer development. To understand the mechanism of how those mutations cause defects in protein function, a point mutation found in XPV patients was introduced in the catalytic core (1-432 amino acids) of hPol $\eta$  by site-directed mutagenesis. Functional assays were carried out with both, the non-mutated and the mutant polymerase, to assess the degree of functionality of the mutant.

## CHEMISTRY UNDERGRADUATE STUDENTS

### EFFECT OF HUMIC ACIDS ON SPECTROPHOTOMETRIC ANALYSIS OF Hg(II) USING DITHIZONE

Zachary Andreasen  
Faculty Research Advisor: Dr. Hong Zhang

Hg (II) can be analyzed spectrophotometrically using dithizone, which has thio-groups of high affinity for Hg(II). Our previous research indicated that humic substances may affect the spectrophotometric analysis of environmental samples of Hg (II). A follow-up investigation was carried out to further quantify this effect using two humic acids, Acros humic acid (ACHA) and Aldrich humic acid (ADHA), together with model organic acids, oxalate and cysteine. Our study shows that both ACHA and ADHA can decrease the sensitivity of the Hg (II) analysis (the slope of the Hg (II) calibration curve) linearly within 20 -80 ppm of the HAs but at 100 ppm; ADHA causes more decrease than ACHA. Compared to the HAs, oxalate only shows a very mild effect over 20-100 ppm. Cysteine shows no effect below 1 ppm, but significantly decreases the calibration curve slopes in a linear manner at 1-3 ppm and completely inhibits the binding of dithizone to Hg (II) above 3 ppm. These results further indicate that the thio-groups in the HAs are responsible for the effect of the HAs on the Hg (II) analysis.

### ANTI-CANCER PROPERTIES OF A NEW SERIES OF ACETYL-ETHYL-PYRAZINE THIOSEMICARBAZONES

Alexandra Arriaga and Dr. Edward C. Lisic  
Faculty Research Advisor: Dr. Edward C. Lisic

Thiosemicarbazone compounds are a class of multidentate ligands that contain potential binding sites for a wide variety of metal ions such as iron and copper. This work will present the synthesis of a series of new, never before synthesized, 2-acetyl-3-ethylpyrazine thiosemicarbazone compounds (AEPZ-TSC's). These new compounds are potential anti-cancer agents, as they most likely interfere with ribonucleotide reductase, an iron-containing enzyme used by cells to produce DNA. They are structurally similar to Triapine, which has undergone Phase 2 clinical trials. The work to be presented includes the structural characterization of the new compounds by <sup>1</sup>H NMR (Nuclear Magnetic Resonance) spectroscopy. The purpose of this project was to synthesize, characterize, and determine the minimum inhibitory concentration (MIC) of this series of compounds for four bacteria (*Bacillus subtilis*, *Staphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa*), two yeast

(*Candida albicans* and *Saccharomyces cerevisiae*), and a mold (*Aspergillus niger*) to determine the indication of biological activity and anti-proliferation capacity.

### SYNTHESIS AND ANTIMICROBIAL STUDIES OF ACETILPYRAZINE-THIOSEMICARBAZONE (APZ-TSC) LIGANDS

Christine Beck, Kathleen Mansour, and Carrie Thompson  
Faculty Research Advisor: Dr. Edward C. Lisic

Several new acetylpyrazine thiosemicarbazone ligands have been synthesized in our laboratory and characterized by <sup>1</sup>H NMR spectrometry. These new compounds have been shown to ligate transition metals such as Pd<sup>2+</sup> and Cu<sup>2+</sup> through an N-N-S tridentate system. These biologically active compounds were tested for antimicrobial activity by determining the minimum inhibitory concentrations against four bacteria (*Bacillus subtilis*, *Saphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa*), two yeast (*Canida albicans* and *Sacchromyces cervisiae*), and one mold (*Aspergillus niger*). Tests show that the Cu<sup>2+</sup> and Pd<sup>2+</sup> complexes of these ligands exhibit different activities than the individual ligands.

### DETERMINATION OF PKA VALUES FOR SYNTHESIZED THIOSEMICARBAZONE AND SEMICARBAZONE LIGANDS

Jacob Buckner and Dr. Amanda Crook  
Faculty Research Advisors: Dr. Dale Ensor  
and Dr. Amanda Crook

Thiosemicarbazone and semicarbazone compounds have been extensively reported in scientific literature. These compounds are used as chelating agents and are being tested as possible cancer fighting agents. This research serves to determine the pKa values of the hydrazinic proton. This proton must be removed prior to metal chelation. These values provide valuable information in determining what pH range these compounds will be most effective at remediating metal ions out of aqueous solutions. This allows selection of ligands that will be successful in chelating metal ions out of natural water supplies at environmental pH ranges. These determinations will be conducted using spectroscopic methods that determine changes between protonated and deprotonated forms of the ligand as pH is varied. This class of compounds is expected to be effective in the pH range of natural water supplies, as preliminary data places the pKa values of the compounds in the range of pH 8.

## TESTING OF ETHANOL AND OF METHANOL IN BRADFORD REAGENT

Brent Cooper, Logan Boles, and Czarinna Clay  
Faculty Research Advisor: Dr. Jeffrey O. Boles

The Bradford Dye binding assay is one of the most prominent and cited assays for determining protein concentration. It exploits a shift in absorbance of Commassie Brilliant Blue to a maximum absorbance of 595 nm when it interacts with protein. The nature of the interaction with protein is unknown. Three different preparations of the Bradford Reagent were utilized in this study in order to determine which provided the strongest and most linear response in preparing standard curves to be used for determining unknown protein concentrations. Commercial Bradford reagent was used, as well as dye preparations with either ethanol or methanol as the primary solvent. Two different proteins were used in this analysis. The results of the study will be presented.

## DETECTION OF METAL IONS USING A PAPER BASED SENSOR

Jamie Dillon, Tyler Thompson, and Daniel Hart  
Faculty Research Advisor: Dr. Andrew Callender

The recreational use of methamphetamines is a growing problem in America, and law enforcement agencies are looking for new and inventive ways of combating this issue. To assist police in solving this problem, we have begun researching ways of identifying the reducing agents used in the production of methamphetamines. Finding a systematic way to quickly identify these will assist in the identification of the producer of the drugs, thus defeating the problem at its root. The reducing agents used to produce methamphetamines are typically metals; therefore, a compleximetric method of identifying them is needed. The simplest and most efficient way of doing so is with a piece of paper that has been dipped in an identifying complexing agent and dried. It is similar in use to that of litmus paper, which detects acidity or basicity of a sample. However, instead of a color change occurring due to hydronium or hydroxide ion presence, the paper strips will change colors based on the presence of a metal ion.

## EFFECT OF MUTATIONS IN DNA POLYMERASE ETA IN XERODERMA PIGMENTOSUM-VARIANT PATIENTS

Joshua Escue and Dr. Xiaohua Jiang  
Faculty Research Advisor: Dr. Xiaohua Jiang

Xeroderma pigmentosum (XP) is a rare autosomal recessive disease in which there is extreme sensitivity to sunlight,

specifically ultra violet radiation. The UV waves cause pyridimine dimers to form between adjacent nucleotides. When DNA is replicating it needs the help of DNA polymerase eta (pol $\eta$ ) to replicate past the dimers. Patients with XP have mutations in their gene coding for DNA led to conformational changes in DNA polymerase eta. These conformational changes lead to a loss of function and are the specific problem that is being researched. By isolating specific mutations in the DNA polymerase gene and creating the protein we hope to learn a great deal about structural changes, especially ones dealing with the catalytic core.

## DIFFERENTIAL PROTEOMIC APPROACH DETERMINING EFFECTS OF THIOSEMICARBAZONES ON CELLULAR MECHANISMS OF TETRAHYMENA

Terra M. Gray and Dr. Sri Bharat Madireddy  
Faculty Research Advisors: Dr. Edward C. Lisic and Dr. Sri Bharat Madireddy

Cancer, defined as the uncontrolled growth of abnormal cells in the body, is the second-leading cause of death in the United States. Current research is shedding light on the potential anti-cancer properties of Thiosemicarbazones (TSCs) as cell growth-inhibitors, bringing science closer than ever before to understanding the mechanisms behind inhibiting, and even curing cancer. The goal of our group's research project is to perform a differential proteomic study in order to propose the cellular mechanisms involved during the drug-exposure. Tetrahymena thermophila SB210 is selected by our group as the model organism to determine the mechanism of action of selected TSC. The proposed research plan will utilize a bottom-up differential proteomic approach in which a two-dimensional gel electrophoresis method is employed to separate the differentially expressed proteins. The up-regulated and down-regulated proteins within the control gel and test gel are subjected to enzymatic digestion, thereby producing peptide fragments. The cluster of peptide fragments from each protein will be subjected to high resolution mass spectrometric analysis. The resulting tandem mass spectrum (MS/MS spectrum) will provide a list of peptides identified and an online protein database search will be used to match the identified peptides to the most probable protein. By achieving a proper proteomic analysis we intend to reveal the cellular mechanisms of anti-cancer properties of the selected TSCs for further study. This vital intermediate step will refine the anti-cancer results previously established by Dr. Edward Lisic's research group at TTU and determine the best TSC candidate for future testing.

## SERIES OF ALLOXAN THIOSEMICARBAZONES: STRUCTURES AND REACTIONS WITH COPPER (II)

Margarett Holder  
Faculty Research Advisor: Dr. Edward C. Lisic

This work demonstrates the synthesis of a series of seven alloxan thiosemicarbazone compounds, and the x-ray crystal structure of one, the alloxan tert-butylthiosemicarbazone. The alloxan substrate was reacted with thiosemicarbazide, 4-methyl-3-thiosemicarbazide, 4-ethyl-3-thiosemicarbazide, 4-tert-butyl-3-thiosemicarbazide, 4-benzyl-3-thiosemicarbazide, 4,4-dimethyl-3-thiosemicarbazide, and 4-phenyl-3thiosemicarbazide to form the thiosemicarbazone ligands. These ligands act as a chelating tridentate ligands with Cu (II) when reacted with copper (II) chloride. These new metal complexes were then tested for anti-proliferative activity in a bacteria study to determine the minimum inhibitory concentrations needed to stop their growth.

## SYNTHESIS OF PYRUALDEHYDE THIOSEMICARBAZONE COMPOUNDS

Amanda Koch, Christy Beck, and Victoria Holcolmb  
Faculty Research Advisor: Dr. Edward C. Lisic

Pyruvaldehyde was reacted with six different thiosemicarbazide compounds to give a series of six compounds. These compounds were characterized by 1H NMR. The five compounds produced are: Pyruvaldehyde Bisphenylthiosemicarbazone, Pyruvaldehyde Bisthiosemicarbazone, Pyruvaldehyde Bisethylthiosemicarbazone, Pyruvaldehyde Dimethylthiosemicarbazone, Pyruvaldehyde Benzilthiosemicarbazone, and Pyruvaldehyde Turtbutylthiosemicarbazone. These compounds will be synthesized with various metals to form metal complexes and then tested to prove or disprove biological benefits. The antimicrobial activity of the previously synthesized pyruvaldehyde thiosemicarbazones and the metal complexes of these compounds will be tested by determining the minimum inhibitory concentrations against four bacteria (*Bacillus subtilis*, *Saphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa*), two yeast (*Canida albicans* and *Sacchromyces cervisiae*), and two molds (*Aspergillus niger* and *Penicillum notam*).

## SYNTHESIS OF A SERIES OF COPPER(II) QUINOLINE-2-CARBOXALDEHYDE THIOSEMICARBAZONE COMPOUNDS

Lizzie Monroe, Dr. Edward C. Lisic, and Sandra Miselem  
Faculty Research Advisor: Dr. Edward C. Lisic

Thiosemicarbazones have significant biological activity as anti-tumor, anti-microbial, and anti-viral agents, often enhanced when complexed with certain transition metals, such as copper. Quinoline-2carboxaldehyde has been used as a substrate to form quinoline-2-carboxaldehyde thiosemicarbazones, QCA-TSC. We present the synthesis and 1H NMR characterization out of seven new QCA-TSC's. These compounds have been reacted with copper to form seven new square planar metal complexes where the QCA-TSC ligands act as chelating ligands.

## SOLAR OVENS TO POWER SIMPLE ORGANIC REACTIONS

Heather Murray  
Faculty Research Advisor: Dr. Daniel J. Swartling

Food will cook in a parabolic solar oven of varying size, given a modicum of solar energy. Given this example, it should follow that parabolic solar ovens could also power a variety of basic chemistry reactions. Reactions successfully run in over the summer of 2012 at Tennessee Technological University include experiments in boiling water to a simple distillation reaction of water and ethanol, with variations in parabolic oven type. These experiments provided exciting results in temperature versus time graphing. Distillation was very satisfactory, running at a reasonable and even rate and providing large samples of separated ethanol. Solar-powered reaction times seemed not dependent on amount of cloud cover as much as available solar wattage, but also seemed dependable so long as there was less than approximately 50% cloud cover in what was a wet summer for the area.

## PROGRESS TOWARDS THE ENANTIOSELECTIVE TOTAL SYNTHESIS OF HAMIGEROMYCIN B

Michael Probasco and John Kirby  
Faculty Research Advisor: Dr. Jesse Carrick

Hamigeromycin B is an aromatic natural product bearing substantial acetogenic character isolated as a secondary metabolite from the soil fungus *Hamigera avellanea* in 2008. Extensive spectroscopic studies were utilized to establish the proposed relative stereochemistry of the target. Biological activity of the resorcylic lactone class of natural products is diverse including targets that display anti-malarial activity as well as cytotoxicity. Progress towards the convergent asymmetric synthesis of this molecule will be presented.

GREEN CHEMISTRY: CHOLINE CHLORIDE  
UREA IN ALDOL CONDENSATIONS

Susannah Claire Shissler  
Faculty Research Advisor: Dr. Daniel J. Swartling

Aldol condensations are integral to the everyday lives of humans because they are commonly used to make ubiquitous items. Aldol condensations have the ability to form carbon-carbon bonds and their products make solvents and plasticizers and are an important intermediate step in many perfumes and pharmaceuticals. One traditional solvent for this reaction is ethanol which has been ridiculed for its environmental impact. Because of the wide-spread use of aldol condensations in industry, the possibility of replacing ethanol is significant. One possible replacement is the deep eutectic solvent choline chloride urea which is reusable and environmentally friendly to produce and use. The purpose of this study is to ascertain the effectiveness of replacing ethanol with choline chloride urea in a couple of general aldol condensations and determine whether the procedure can be fine-tuned to make a better product. Its effectiveness will be determined by comparing the yields of the different solvents.

DISTRIBUTION OF SODIUM USING  
THE NEXT-GENERATION CAUSTIC-SIDE  
SOLVENT EXTRACTION

Christopher Shults  
Faculty Research Advisor: Dr. Dale Ensor

The Next-Generation Caustic-Side Solvent Extraction (NG-CSSX) has been developed to enhance the ability to remove radioactive cesium from alkaline salt waste. This legacy waste from the Cold War is currently stored at the Savannah River Site and must be decontaminated before disposal. The components of the system include the extractant molecule known as MaxCalix, a modifier, Cs-7SB, that helps increase the solubility of MaxCalix and prevents the formation of a third phase during extraction, using the commercial solvent, Isopar<sup>®</sup> as the diluent. A significant amount of data has been generated on the effects of anions (NO<sub>3</sub><sup>-</sup>, NO<sub>2</sub><sup>-</sup>, and OH<sup>-</sup>) on the cesium distribution ratio using NGCSSX. In order to better understand the extraction mechanism the behavior of sodium ion, a major interference to the extraction of cesium, must be characterized. Sodium distribution under a variety of conditions has been measured by a radiotracer method. This new information combined with previous data has allowed the development of a better understanding of the NG-CSSX system.

DESIGN AND PRESENTATION OF  
INTERACTIVE VSEPR THEORY VIDEO

Haley Snyder, Mrs. Janet Coonce, and Dr. Scott Northrup  
Faculty Research Advisors: Mrs. Janet Coonce  
and Dr. Scott Northrup

The Valence Shell Electron Pair Repulsion (VSEPR) theory is important in the study of chemistry, but it is often not fully grasped by general chemistry students. As an aid for visualizing this theory, a ten minute educational video was created with an accompanying handout to supplement course activities. The hypothesis for this project is that students who are shown a short video while interacting with the accompanying handout will perform better on related quiz questions than students who are shown the video without the handout. All students (NT=479) in a total of 9 STEM major undergraduate chemistry laboratory sections were given a short lecture presentation before performing a hands-on VSEPR model building activity. Students were assigned to three treatment groups. Group A (NA=160) was shown the video with an accompanying handout, Group B (NB=165) was shown the supplemental video without the handout, and the Control Group (NC=154) were neither shown the video nor given the handout. Group A was found to score higher on a subsequent quiz than those in either Group B or the Control Group. Group B performed better on the quiz that followed than the Control Group.

RESOLVING THE BACTERIAL  
SELENOMETHIONYL PROTEOME  
FOR DIFFERENTIAL EXPRESSION  
PROTEOMIC ANALYSIS

Savannah J. Taylor, Kathleen M. Broderick,  
and Dr. Jeffrey O. Boles  
Faculty Research Advisor: Dr. Jeffrey O. Boles

When incorporated into proteins, selenomethionine (SeMet) is a useful tool for many researchers to investigate the structure (and consequently the function) of proteins in natural systems. Even though SeMet can be incorporated into most bacterial proteins and allows cell division to proceed albeit at a much slower rate, it cannot be incorporated into all proteins without disrupting activity and/or structure. Using two dimensional electrophoresis, the identification of differentially expressed selenomethionyl proteins was compared to wild type Escherichia Coli proteins to provide insight into the cause of depressed cell growth rates. This molecular level information could lead to a solution of the toxicity problem via altered growth media or metabolically engineered strains once the function of the differentially expressed proteins are determined.

## CHROMATOGRAPHIC MATERIAL FOR THE SEPARATION OF MINOR ACTINIDES FROM LANTHANIDES

Kayron Tevepaugh  
Faculty Research Advisor: Dr. Dale Ensor

The elements americium and curium (actinides) and europium (lanthanide) are fission products in the nation's spent nuclear reactor fuel used for electrical power generation. Interest in separating these lanthanides from actinides is increasing due to the growing necessity to manage the geologic repositories of radioactive materials. This particular separation is a key step in minimizing the amount of spent nuclear fuels requiring long term storage. One way to achieve this is via a chromatographic column, an open tube packed with small resin particles that have been loaded with a compound having the ability to retain actinides on the column while the lanthanides flow through, thus separating these elements. Camphor-BTP is a compound that has shown the ability to accomplish this particular separation. The procedure involves loading the Camphor-BTP onto the small resin particles and then exposing the resin to americium and europium separately to assess the activity retained by the material. Results showed that Camphor-BTP illustrated a strong preference for americium over europium, indicating that the europium should flow through the column quickly and separate from the americium which will flow through the column slowly. Column experiments have been performed that show efficient separation of americium from europium.

## STRUCTURES AND BACTERIA STUDIES OF FORMYLCHROMONE THIOSEMICARBAZONES AND THEIR METAL COMPLEXES

Amanda Werlein and Kathleen Mansour  
Faculty Research Advisor: Dr. Edward C. Lisic

Thiosemicarbazone compounds are potent biological agents, and they can also act as ligands to form copper (II) complexes. A series of semicarbazone and thiosemicarbazone compounds synthesized from a formylchromone backbone in our laboratory will be presented. The synthesis of this series of compounds is straightforward, and characterization by <sup>1</sup>H NMR and IR supports the proposed structures. Research efforts to synthesize the copper (II) complexes will also be discussed.

## EARTH SCIENCES UNDERGRADUATE STUDENTS

### MEASURING LAG TIMES AND SUSPENDED SEDIMENT CONCENTRATION IN AN URBANIZED KARST WATERSHED

Kolbe Andrzejewski and Dr. Evan Hart  
Faculty Research Advisor: Dr. Evan Hart

The city of Cookeville, TN lies within a karst watershed where the city's stormwater runoff passes through a series of sinkholes and caves. Sinkhole flooding is a common occurrence in the city and floodplains have been delineated for over 200 sinkholes. Sinkhole flooding occurs when runoff arrives to the sinkhole at a rate that exceeds the drainage rate out of the sinkhole. Sinkhole drainage rates and relationships between rainfall and sinkhole flooding have been determined by previous research. However, the effects of sinkholes and caves on downstream flood stages and lag times have not been studied. We hypothesize that sinkholes act as detention basins, reducing peak runoff rates. The cave system below the sinkholes may also act as a storage reservoir during floods. To test this hypothesis, we instrumented sinkholes, the cave, and downstream resurgence points with automatic stage recorders to determine lag times through the cave. For comparison, we also instrumented and measured lag times in a neighboring watershed without a cave. We also measured suspended sediment concentrations at these locations in order to determine the effects of the cave on sediment transport. Preliminary results indicate lag times between 200 and 330 minutes for the cave stream and between 25 and 65 minutes for the non-cave stream. Suspended sediment concentrations ranged from 200 to 1800 mg/l for both the cave stream and non-cave stream systems. These results indicate that lag times are longer for the cave stream, however, suspended sediment concentrations are similar for both stream systems.

### DETERMINING FLOOD-PRONE AREAS WITHIN WHITE COUNTY PARKS USING SCS METHOD

Jonathan Andrew DiOrio  
Faculty Research Advisor: Dr. Peter Li

Both the Virgin Falls Natural State Area and Bridgestone/Firestone Centennial Wilderness Area can be found in the greater Scott's Gulf region of Tennessee, which is located in the southeastern corner of White County. These two areas combined cover approximately 14,384 acres of largely undeveloped deciduous forest, and are visited year round

by hikers, cavers, environmental scientists, and many others for its waterfalls, caves, overlooks and karst-rich sinkholes, which are characteristically found in the Cumberland Plateau area. However, according to the Tennessee Department of Environment and Conservation as well as the Tennessee Wildlife Resources Agency, the streams within these two areas are prone to flash flooding, which poses a large potential hazard for any unfortunate individual(s) who might find themselves along trails or campsites that are within a relatively close proximity these streams when disaster strikes. This study utilizes the SCS method, which incorporates data layers such as land use, soil types, watersheds, elevation/slope, and precipitation records of the area (as well as other data) to estimate runoff peak volumes during various precipitation events. The curve numbers are developed based on soil types and land use patterns in the area. The average curve number that is derived from these GIS calculations is used to estimate the likely runoff volume in the study area, as well as allow us to deduce which areas will become most affected by flash flooding. The results of this study will be provided to those who manage the area for aid in future policy making.

## RUNOFF MODELING FOR AN URBAN STREAM IN COOKEVILLE, TN

Joseph Ellis  
Faculty Research Advisor: Dr. Evan Hart

A runoff model was developed for Denton Creek (201 acres), an urbanized stream in Cookeville; TN. Denton Creek drains residential and commercial areas including a portion of the Tennessee Tech campus. Development of a runoff model for Denton Creek is important in light of recent flooding in the watershed. In 2010, floodwaters nearly flooded a medical office building under which Denton Creek passes via a culvert. Denton Creek also commonly floods a large sinkhole in a residential neighborhood. For these reasons, a runoff model for Denton Creek will be useful for future flood mitigation projects. Win-TR55 (US Army Corps of Engineers) was used to develop the runoff model. Watershed data for model input included drainage area, land use, impervious area, soil type, surface roughness, and flow path length. Channel data included channel dimensions, slope, and channel roughness. In order to validate model results, we installed a HOBO water level logger at a bridge culvert to record stage data at 5 min intervals. Rainfall data were obtained from the Kittrell Hall rain gauge, in the northern part of the watershed. Land use data were obtained by digitizing air photos using GIS software. Land uses were as follows: impervious surfaces 35%, lawns/open space 30%, and woods 35%. Model results predict a time of concentration of 0.30 hr and peak discharges for the 2, 10, and 100 year -24 hour rain events to be 350 cfs, 620 cfs, and 1000 cfs, respectively. Observed stage data fit closely with

model results, however more observed data is needed to increase model confidence.

## ANALYSIS OF QUARTZ-CLAST SIZE DISTRIBUTION IN ANCIENT TERRACE DEPOSITS, PUTNAM COUNTY, TN

Geoffrey T. Gadd  
Faculty Research Advisor: Dr. Michael Harrison

The Waynesboro Series is a soil deposit that can be found on the Highland Rim of middle TN. The Waynesboro is characterized by deep, well-drained, reddish soils that form ancient terraces located high above modern terraces. Within the Waynesboro, rounded quartz granules and pebbles are present. These quartz clasts were eroded from the Pennsylvanian-aged sandstone on the Cumberland Plateau and then transported by more recent streams. In this study, quartz-clast size was measured to assess the flow direction of the streams that formed the ancient terraces. Quartz clasts were separated from the soil matrix using wet sieving; then the quartz clasts were dry sieved to sort them by grain size. The weight of the quartz clasts was measured for each grain size and then compared to the cumulative weight. A map was constructed to show the quartz-clast distribution. Preliminary results suggest that quartz-clast size decreases with distance from the Cumberland Plateau, indicating a westward stream-flow direction for the ancient terrace deposits.

## MESOSCOPIC STRUCTURES OF POND GULF, NEAR DUNLAP, TN

Joseph Kalbarczyk  
Faculty Research Advisor: Dr. Michael Harrison

Newly discovered tectonic structures in the Pond Gulf area of the Brockdell Quadrangle provide additional information on the lateral extent of the Alleghanian Sequatchie Valley Fault. A structural analysis of Pond Gulf shows a deformation style that is similar to structures exposed ~5 km to the southwest along TN111/8 near Dunlap, TN. The faults and folds in Pond Gulf developed in Pennsylvanian-age clastics and they are associated with Alleghanian compression and extension. The folds within Pond Gulf show cm-scale folding that resulted from hanging-wall deformation of the Sequatchie Valley Fault. Normal faults striking ~060 indicate extension during or after compression. This discovery of faults and folds along the northwest limb of the Sequatchie Valley anticline provides new clues to the timing and extent of the Sequatchie Valley detachment.

## CHARACTERISTICS OF BEDLOAD IN A KARST STREAM SYSTEM

Kyle Long

Faculty Research Advisor: Dr. Evan Hart

Despite the widespread occurrence of karst terrain, few studies have examined bedload transport in caves. Bedload size and roundness are likely to be affected by abrasion inside caves. This study examines bedload characteristics including size, roundness, and lithology in the Pigeon Roost watershed, Cookeville, TN. Data were collected from stream reaches upstream from, within, and downstream from Capshaw Cave. Data were also collected from a control stream, Hudgens Creek, which does not flow through a cave. Nine random samples were taken from within Capshaw Cave, six at the resurgence, and 6 from the swallet and 4 random samples were taken from Hudgens creek. Samples were also collected along the length of Hudgens Creek, the control stream. Samples were processed through sieves ranging from 5.6mm to 25mm. Clasts were examined for degree of rounding or angularity and for lithology (acid test for limestone). Nine roundness classes were recognized. Particle size for samples along Hudgens Creek were smaller and had a lower mean roundness (4.0) than Capshaw Cave stream (6.6). The higher the number the rounder the bedload is. These results show that before streams enter the cave, the sediments are more angular and rapidly become rounded within the cave. Bedload in the control stream does not show the same rate of downstream rounding. Thus, bedload in karst watersheds may have greater transport distances due to smaller particles sizes. For both streams, fewer than 10% of all particles were limestone and most were chert, but no difference was found in lithology between the two study streams.

## A COMPARISON OF MAGNETIC MINERALS IN MODERN AND PLEISTOCENE AGED WIND BLOWN DEPOSITS

Chelsea Ottenfeld

Faculty Research Advisor: Dr. Michael Harrison

Collaborators: Kimberly Yauk (University of Minnesota-Twin Cities) and Bruce Moskowitz (University of Minnesota-Twin Cities)

During the last ice age, the Laurentide Ice Sheet advanced south into the U.S. Midcontinent and windblown dust deposits called loess accumulated adjacent to the Mississippi River. Presently, storms in the southwestern U.S. are depositing dust on snowpack and the iron minerals are changing the albedo of the snow. This study investigated the iron-mineral content of ancient and modern wind-blown dust by using magnetic analysis. Magnetic analysis

is advantageous because it is non-destructive and it can detect low abundance (<1 wt%) and small grain sizes (<100nm). Modern dust samples from Arizona and Utah show a goethite/hematite ratio range of 0.07-0.3. In the Mississippi River Valley of west Tennessee, two Pleistocene loess units were sampled: the Peoria Loess and the Roxana Loess. Preliminary magnetic susceptibility measurements and Munsell color classification of the loess indicates the presence of ferromagnetic minerals. Average magnetic susceptibility values for the Roxana and Peoria Loess deposits are  $0.102 \times 10^{-3}$  SI and  $0.516 \times 10^{-3}$  SI, respectively. These values are similar to Pleistocene deposits from Europe and Asia.

## ANALYSIS OF LAND USE/LAND COVER, SOIL LOSS, AND RUNOFF ON MILITARY INSTALLATIONS

Kaylee Marie Radzysinski

Faculty Research Advisor: Dr. Peter Li

Military training can have adverse effects on Land Use/Land Cover (LULC), soil loss, and runoff. This hypothesis is based mainly on my experience utilizing a small area on Tennessee Tech's campus, referred to as TA1, in ROTC for the duration of the last 4 years. Increased activity on an area of land not only changes the LULC status, but it also decreases soil loss, and increases runoff. From analyzing the LULC and soil data layers I will derive a soil loss equation (RUSLE) in order to predict the effects of military training on three military posts located in the Southeast. These posts are; Fort Campbell located in Kentucky, Fort Bragg located in North Carolina, and Fort Benning located in Georgia. After assessing the degree of change that takes place the new Land Use/Land Cover type, soil loss amount, and runoff amount will be identified given a particular precipitation event for a given amount of time.

## USE OF GIS FOR SUSTAINABLE AGRICULTURE

Stuart Richey

Faculty Research Advisor: Dr. Peter Li

The purpose of this study is to find the most suitable land for sustainable farming using functions and geodatabase structures in GIS. Feature datasets and classes such as digital elevation models, soil types, transportation networks, land use land cover patterns, demographic data, political boundary, and climate data will be built into geodatabase to create base map. The study will investigate soil loss from each suitable land, in combining with other factors, such as land value, proximity to major cities, and pH values of individual soil types to determine the final candidate for building sustainable agricultural land in Tennessee. Flood

scenarios will be simulated to find the peak flow volume in different rainfall events. Watershed delineation processes will create local watershed to help the scope of study area. Water resources information is another important factor in finding the suitable land. Final layers will come from models created from the above information.

## DESCRIPTIVE ANALYSIS OF JOINTS: BROWNS GAP QUARRY, TN

Jordan Sachs and John Baird  
Faculty Research Advisor: Dr. Michael Harrison

The Mississippian Bangor Limestone at Brown Gap Quarry in the Sequatchie Valley shows two orthogonal joint sets oriented northwest and northeast. Within orogenic forelands, cross-strike joints often represent a regional maximum horizontal-stress trajectory formed by syntectonic hydrofracturing. Strike-parallel joints generally reflect outer-arc extension of folded rock layers. At Brown Gap Quarry, syntectonic hydrofracturing is suggested by carbonate mineralization of the cross-strike joints. Outer-arc extension is indicated by the parallelism of the northeast-striking joints and the fold hinge of the Sequatchie Valley anticline. Since calcite, a diamagnetic mineral, is the dominant vein mineral, it was hypothesized that the magnetic susceptibility of mineralized joints would be less than non-mineralized joints. However, it was determined using a t-test that there was no significant difference in magnetic susceptibility between the two joint sets. Since data were collected throughout the year, the effect of seasonal temperature on magnetic susceptibility was assessed. An inverse relationship between susceptibility and temperature was found for all samples; furthermore, for the mineralized joints, the susceptibility decreased at twice the rate than the non-mineralized samples.

## AGE AND CORRELATION BY CONODONTS OF NEWLY DISCOVERED LIMESTONES FROM CENTRAL TENNESSEE

Phillip Van Dervort  
Faculty Research Advisor: Dr. Larry Knox

An interval containing two limestone beds along Interstate 65 occurs some 30 miles north of the Tennessee-Alabama state line. These two limestone beds are truncated above by an erosional surface and have not been recognized in any other part of central Tennessee. Because of their unique occurrence they were sampled for conodonts in order to determine their age. Conodonts from the two limestone beds were identified to genus and species level. Seven species of *Siphonodella* and one species of *Gnathodus* were found in the two limestone units. The

species include *S. duplicata*, *S. quadruplicata*, *S. cooperi*, *S. obsoleta*, *S. sulcata*, *S. crenulata* and *Gnathodus delicatus*. The conodonts are tentatively assigned to the *Siphonodella quadruplicata*-*S. crenulata* Zone of Collinson, Scott and Rexroad, 1962. This zone has been reported from the upper Hannibal and lowermost Chouteau Formations of the Mississippi Valley, and their conodont fauna confirms their unusual stratigraphic occurrence. They represent the oldest Mississippian limestone beds that have been reported from central Tennessee.

## DISTINGUISHING K-BENTONITES USING SCANNING ELECTRON MICROSCOPE AND X-RAY FLUORESCENCE FOR FURTHER RESOLUTION

Paul Woods  
Faculty Research Advisor: Dr. H. Wayne Leimer

David Buhl performed analysis of known and unknown K-Bentonites using the petrographic microscope and clay examination though the use of X-ray Diffraction, this study was to identify different beds of K-Bentonites. Identification was made from diagnostic mineral phenocrysts that are characteristic to the Deike (T-3) and Millbrig (T-4). Each K-Bentonite represents independent volcanic ash fall events that occurred 450-460 million years ago during the Ordovician. The volcanic ash beds have been altered into K-Bentonites. Deike and Millbrig control samples were supplied from Nyrstar NV exploration cores. These contained known sequences of T-3, T-4, and T-5. Field samples were collected along a forty-five mile long section of the Kingston Thrust sheet from Oak Ridge, TN. and north of Decatur, TN. Further analysis of K-Bentonites thin section will use the Scanning Electron Microscope (SEM) and X-ray Fluorescence (XRF). The SEM primary use is to locate diagnostic plagioclase phenocrysts. The XRF will provide a 'whole rock' analysis in weight percent oxides (WT %). The SEM will use spot scanning to scan the background clay component, and see if there are any plagioclase crystals present (labradorite for T-3, andesine for T-4). Results from the XRF will be a 'whole rock' quantification to view if there is any variance between the known samplings in WT%. The comparison between known and unknown samples will be used to help bring a better resolution, and determined which tool would be most appropriate for further analysis of K-Bentonites.

## ENVIRONMENTAL SCIENCES GRADUATE STUDENTS

### DEVELOPMENT OF A SOLAR REFLECTOR FOR USE IN ORGANIC SYNTHESIS REACTIONS

Brian M. Agee and Dr. Daniel J. Swartling  
Faculty Research Advisor: Dr. Daniel J. Swartling

Since the 1990's, scientists have been attempting to make chemical synthesis procedures more environmentally friendly. One area of environmental concern is the amount of electricity required to provide enough energy to complete an experiment. An effective means for lowering the electricity needed to drive chemical reactions to completion is proposed through the use of solar parabolic reflectors. These solar reflectors are assembled by covering unused satellite dishes with Mylar® tape. This gives the satellite dish reflective properties when the dish is directed at the sun. Preliminary research has shown that the solar reflector is capable of heating a substance to a temperature over 300°C. This temperature is more than capable to drive most organic synthesis reactions to completion. The ability to use the solar reflector as the sole heat source for organic synthesis reactions such as Friedel-Crafts acylation reactions and Wolff-Kishner reduction reactions is being investigated. Comparative studies were conducted using an electrical heat source to compare the solar reflectors ability to generate heat to drive the chemical reactions to completion. Analysis of the products of the reactions will be performed using NMR.

### DIFFERENTIAL PROTEOMIC STUDY TO DETERMINE THE SUB-LETHAL EFFECTS OF GOLD NANOPARTICLES ON TETRAHYMENA

Vanaja Reddy Bodeddula and Dr. Sri Bharat Madireddy  
Faculty Research Advisor: Dr. Jeffrey O. Boles  
Collaborator: Dr. Sharon G. Berk

Recent reports indicate that nanoparticles present in various man-made products are being released into the aquatic environment. Exposures to nanoparticles lead to numerous biological and toxicological effects in aquatic organisms. A differential expression proteomic strategy was selected to examine the effects of nanoparticles on living organisms. The test organism used in this research is a strain of *Tetrahymena*, a widely used unicellular eukaryotic ciliated protozoan. Protozoans are one of the easiest organisms that can be studied to determine the effect of nanoparticles

on a proteome. In this study, two sets of *Tetrahymena* sp. cells were cultured, where one was exposed to 20nm unconjugated gold nanoparticles. Proteins from the two cultures were extracted and separated by two-dimensional electrophoresis (first dimension isoelectric focusing and second dimension sodium dodecyl sulfate polyacrylamide gel electrophoresis) maintaining the same set of conditions for both control and test cultures. After performing duplicate exposures, six up-regulated proteins involved in stress-related conditions, electron transport system and tri-carboxylic acid cycle, ribosomal translocation during protein synthesis and calcium binding processes. Eight down-regulated proteins involved in ATPase activity, methyl citrate cycle, ribosome biogenesis, granule regeneration and one-carbon metabolic process were identified by nano-electrospray ionization quadrupole time-of-flight mass spectrometry, followed by protein identification using online protein databases ProteinLynx Global Server and MASCOT. Triplicate exposures resulted in three up-regulated and five down-regulated proteins. Stress-related proteins were found to be up-regulated. The down-regulated proteins were involved in ATPase activity, ATP binding, 2-methylcitrate pathway, ribosome biogenesis (catalytic process), oxidoreductase activity and granule regeneration.

### NEW CRAYFISH DIVERSITY IN THE COLLINS RIVER DRAINAGE OF TENNESSEE

John W. Johansen, Dr. Hayden T. Mattingly,  
and Brianna C. Zuber  
Faculty Research Advisor: Dr. Hayden T. Mattingly

Tennessee has a diverse crayfish fauna with over 80 described species. Although this rich fauna has been studied for approximately 40 years, many areas of the state still need comprehensive surveys before its true diversity is known. The Collins River contains a unique aquatic fauna including several endemic and imperiled fish and freshwater mussels, but little is known about the crayfish diversity of this drainage. Historically 10 species, including the non-native *Orconectes rusticus*, have been reported from 23 localities. During summer and autumn of 2012, we made several crayfish collections in the Barren Fork. These collections identified two species previously unreported from the Collins River: Brawley's Fork Crayfish, *Cambarus williamsi*, a species thought to be endemic to the neighboring East Fork Stones watershed and an undescribed species of *Orconectes*. Additional surveys should be conducted in the Collins River to document its crayfish diversity and determine the range of *O. rusticus*, *C. williamsi*, and *Orconectes* sp. nov. in the drainage. To properly plan and prioritize conservation efforts, a full understanding of regional diversity and species distributions is necessary.

## NEW DRAINAGE BASIN DISTRIBUTIONAL RECORD FOR BRAWLEY'S FORK CRAYFISH, CAMBARUS WILLIAMI

John W. Johansen and Dr. Hayden T. Mattingly  
 Faculty Research Advisor: Dr. Hayden T. Mattingly  
 Collaborator: David I. Withers (Tennessee Department of Environment and Conservation)

Brawley's Fork Crayfish, *Cambarus williami* is one of more than 80 crayfish species native to Tennessee. Previously thought to be endemic to East Fork Stones River (EFSR) in the Nashville Basin physiographic province, its current AFS status (Endangered) and Heritage rank (G1, S1) are indicative of a restricted range. However, a single Form II male from the Barren Fork of the Collins River was collected in September 2012. The collection site was located in Bullpen Creek in Cannon County, approximately 6.1 air km southeast of the nearest documented EFSR population. Subsequent visits to this stream yielded additional individuals, including Form I males, and indicated that an established population exists in Bullpen Creek. This discovery expands the known range and elevation extent of *C. williami* to a new drainage and physiographic region. We plan to conduct additional surveys of the Collins River to determine the distribution and abundance of *C. williami* within the drainage. Such surveys will be necessary to inform any re-evaluation of the species' current conservation status.

## A PARTICIPATORY PILOT STUDY ON BIOMASS PYROLYSIS: FEEDBACK FROM TWO UPPERCUMBERLAND COUNTIES

Jessica Murillo, Lachelle Norris, and Dr. Joseph J. Biernacki  
 Faculty Research Advisor: Dr. Joseph J. Biernacki  
 Collaborator: Dr. C. Pat Bagley

Government mandates and initiatives have prompted growth in all areas of the renewable energy sector in hopes of attaining national energy security, economic growth, and environmental sustainability. Biomass-based energy is still the only meaningful route for producing liquid fuels. Biomass-based processes are being honed to produce renewable chemicals for the lucrative and ever-expanding byproducts industry to displace petroleum-based products. As processing cellulosic biomass becomes reality, a higher demand for biomass feedstock raises questions about supply logistics and sustainability. The front-runners for biomass feedstock are waste products from agriculture, forestry, and municipalities; and energy crops, such as switchgrass, poplar, and camelina. The important question is who will grow the feedstocks and how will they be compensated for? The farmer, rural community, and agriculture have been left out of the biofuels equation. Therefore 28 farmers

and 15 facilitators from Tennessee farming communities provided information through informal question and answer sessions and through questionnaires. A two-tiered approach gathered information from Scott and Putnam county farmers. To involve those who will be affected by the research, a focus group of 15-20 local conservationists was formed to uncover relevant questions and concerns that local growers have regarding changes brought about by a shift to a biofuels-agro-economy. The result of the focus group was incorporated into a questionnaire administered at District Conservation meetings in Scott and Putnam counties following a biofuels presentation given by the researcher. Many farmers were very aware of first generation biomass feedstock and fuels.

## PHOTOCHEMICAL REDUCTION OF MERCURY(II) BY HUMIC ACID AND UVB AT PH 6-9

Stephen Okine and Dr. Hong Zhang  
 Faculty Research Advisor: Dr. Hong Zhang  
 Collaborator: Dr. Baohua Gu (Oak Ridge National Laboratory, Environmental Sciences Division)

We studied the mechanism and kinetics of photoreduction of Hg(II) by humic acids at pH 6-9 using Hg(II) and commercial Aldrich Humic Acid (AHA) with a photochemical setup (four UVB fluorescence lamps and a quartz tube containing Hg(ClO<sub>4</sub>)<sub>2</sub> and AHA). The concentrations of Hg(II) were followed spectrophotometrically using dithizone over time. We found that 0.6 ppm of Hg(II) was completely reduced in the presence of 2.7 ppm of AHA in 3 h (33.33% Hg(II) reduced/h), and partially reduced with 6 ppm AHA in 6 h (~6.33% Hg(II) reduced/h); but in the presence of 10 ppm AHA, no reduction of Hg(II) occurred over 6 h. The control experiment with no AHA showed only 0.42% Hg(II) was reduced per hour. These findings seem to suggest a dependence of the Hg(II) photo-reduction on AHA, which may induce and favor Hg(II) reduction or Hg(0) oxidation, depending on AHA level.

## MATHEMATICS GRADUATE STUDENTS

### FRACTIONAL CALCULUS AND FRACTIONAL DIFFERENTIAL EQUATIONS

Christopher Hatcher  
 Faculty Research Advisors: Dr. Michael Allen and Dr. Andrew Hetzel

Fractional calculus has been around since the development of modern calculus. However, it has been left mainly unexplored until the end of the 20th century. This paper will provide a survey of fractional calculus and the preliminary

concepts that led up to fractional integrals and derivatives. The end goal is to examine the ways of solving fractional differential equations exactly or numerically. This paper will examine exponentiation beyond integers to include real exponents like pi, square root of 2, and other irrational numbers. The power rule for a monomial of degree n will be broadened to include rational and real exponents. Then power series and power series expansions will be defined and examined at which point, we will show why our common definitions will not hold in fractional calculus. Next, we will take the nth derivative of a general n-times differentiable function using the limit definition. Finally, we will present the Gamma function and useful properties which are essential to solving fractional differ integrals, and Laplace transforms which expand our ability to easily solve fractional differential equations of certain forms. Afterwards, we explicitly define fractional derivatives and integrals along with common properties of fractional derivatives. The paper concludes with discusses creating a fractional differential equations from a second order differential equation and its exact solution, examining various methods for solving fractional differential equations, and where these are used and some examples of simple fractional differential equations and solutions.

## LIKELIHOOD INFERENCE FOR THE GENERALIZED PARETO DISTRIBUTION

Alfredo Ramirez  
Faculty Research Advisor: Dr. David Smith

The generalized Pareto distribution (GPD) can be used to model events that exceed a certain threshold. The GPD can be used in various practical applications such as in meteorology when trying to model unusually long periods of drought. However, in order to successfully apply the GPD to these types of data sets it is important to have a good estimation of the GPD parameters. While various methods exist to estimate these parameters, this paper will focus primarily on constructing interval estimates based on the maximum likelihood (ML). Although ML estimation itself has drawbacks it is the goal of this paper to improve on interval estimation of the GPD parameters using ML.

## PHYSICS UNDERGRADUATE STUDENTS

### WIDTH AND SPACING DISTRIBUTIONS IN NUCLEAR DATA

Travis Johnson  
Faculty Research Advisor: Dr. John Shriner  
Collaborators: Dr. John Shriner and G.E. Mitchell (North Carolina St. University)

A recent study focusing on neutron resonance widths (P. E. Koehler, 2011) has called into question whether the Gaussian orthogonal ensemble (GOE) version of random matrix theory describes nuclear resonance data. The conclusion that the data are inconsistent with GOE seems in contradiction with the analysis of resonance spacing data. We wish to test the possibility that the distribution is not truly GOE but the spacing data by themselves still appear to be described by the GOE. We have simulated both width and spacing distributions that differ by varying amounts from the GOE distribution and determined how one estimate of GOE behavior, the fraction of missing levels, behaves as we deviate increasingly from a GOE distribution. Results will be presented.

## DETECTION OF CORRELATIONS IN STELLAR ISOTOPIC ABUNDANCES

K.A. Thomsen and M.S. Smith  
Faculty Research Advisor: Dr. Raymond Kozub  
Collaborator: Dr. Michael Smith (Oak Ridge National Laboratory)

The composition of a star changes with time via sequences of thermonuclear reactions. These sequences strongly couple the abundances of all elements to each other. The resulting complex interdependencies often make it difficult to ascertain which isotopic abundances most influence one another. To investigate this, a FORTRAN program has been written which analyzes these abundances over time as predicted by a simulation to determine if they may be correlated. This is accomplished via a looping over all possible pairs of tracked isotopes, quantitatively ascertaining the shapes of the abundance versus time curves for each, and assigning numerical scores to determine if these pairs of curves are correlated, anti-Correlated, or uncorrelated. Preliminary results from this study will be presented.

## SOCIOLOGY AND POLITICAL SCIENCE UNDERGRADUATE STUDENT

### INDIVIDUAL ONLINE IDENTITY MANAGEMENT

Amanda Brown  
Faculty Research Advisor: Dr. Lachelle Norris

This study addressed the implications of identity management in a new, technology based society. This paper will apply the question: How do people create and manage their online identity? Elements of impression management on Social Networking Sites, specifically Facebook, will be examined to determine how individuals have adapted to representing themselves online. Impression management

has been sociologically relevant since Goffman first introduced his theory of dramaturgy with the idea of front stage/ back stage in 1959. While Goffman could have never conceived his findings to be relevant in a virtual, online society; the same idea still proves to be ever-present on the notorious Social Network, Facebook. The research proposed here is a qualitative analysis of how individuals maintain their online identity as a separate sphere, to represent themselves alone, through aspects of communications, social interaction, self-presented goals, and self-relevant information. Impression management is ever present in all societies; and understanding how impression management has changed from face-to-face self-representation to online, virtual representation is pertinent to understand how individuals adapt to changing society.

## COUNSELING AND PSYCHOLOGY UNDERGRADUATE STUDENT

### ADDICTION AS A PREDICTOR OF ATTITUDE, MOTIVATION AND, SELF-EFFICACY THROUGH PINTEREST

Samantha Fallos  
Faculty Research Advisor: Dr. Christopher Burgin

The purpose of this experiment was to explore addiction and personality traits of those who use Pinterest to determine pinning content, self-efficacy, and reflection of self. Participants were recruited via Pinterest and Facebook. The sample consisted of 100 females with a mean age of 24.93 (SD = 7.67), who have a Pinterest account. Participants were given a Qualtrics link that led them to complete a series of questionnaires including; the first four sections of the Self-Attributes questionnaire to measure participant's attitudes on their abilities to complete certain tasks, the Big Five Inventory (short), to measure Openness, Conscientiousness, Extraversion, Agreeableness, and Neuroticism, a Pinterest Addiction scale, to measure level of Addiction to the site, a lifestyle questionnaire, to reflect participant's daily activities, a demographic page, and a Pinterest demographic page. The results demonstrate that participants who scored higher on neuroticism and lower on conscientiousness scored significantly higher on the Pinterest Addiction scale than other personality traits ( $p < .05$ ). Higher levels of addiction significantly predicted a longer amount of time spent on the website ( $p < .05$ ), however, there was no significance between level of addiction and the number of pins posted ( $p > .05$ ). In addition, personality variables did not significantly predict variety in pinning content or with the number of liked pins versus reposted pins (both  $p$ 's  $> .05$ ). The findings of the study show support for the different demographics each user brings to the use of Pinterest.

### EXAMINING THE EFFECT OF ISOLATION AND CELL PHONE USE ON STATE ANXIETY

Kelley Garrison  
Faculty Research Advisor: Dr. Matthew Zagumny

The purpose of this experiment is to measure how cell phone use and isolation affect a person's state anxiety. It is hypothesized that participants who are prohibited from using their cell phone will have significantly higher state anxiety than those participants allowed to use their cell phones, regardless of the pairing condition. It is also hypothesized that participants who are waiting in a room alone for a short period of time and are prohibited from using their cell phones will have significantly higher state anxiety than all other groups. Participants were randomly assigned to one of four treatment groups: (1) Waiting alone and allowed to use their cell phone; (2) waiting alone and prohibited from using their cell phone; (3) waiting in pairs and allowed to use their cell phone; or (4) waiting in pairs and prohibited from using their cell phone. After sitting in a room for a five minute period, during which participants' cell phone use was observed by the researcher from an adjoining room through a one-way mirror, they were asked to complete an online version of the State-Trait Anxiety Inventory, assessing their state anxiety and trait anxiety. Sociodemographic information was also collected including gender, age, class standing, cell phone ownership and use, type of cell phone, use of cell phone during the study, how they used their phone during the study, and if participants knew the other participant in the room. Participants were recruited from general education classes at Tennessee Tech University. Study participation was completely anonymous and all data is being collected on the secure Qualtrics server. Preliminary analyses suggest initial support for the research hypotheses. Data collection and preparation of the final manuscript will be complete by mid-April.

### HUMAN AND DOG FACTORS PREDICT DOG APPROACHABILITY

Leah Shulley  
Faculty Research Advisor: Dr. Zachary Wilcox

The Centers for Disease Control (2009) reported that each year over 4.7 million individuals in the United States are bitten by a dog. It is extremely important to understand why these figures are so high. Perceived approachability of dogs is obviously an important factor related to being bitten. Previous researchers have examined factors that influence perceived behavior as well as emotional expressiveness of dogs. However, there has been little research regarding factors that influence perceived approachability of dogs. Data from 330 college students were analyzed to determine

how morphological features of a dog and factors related to the participant affect perceived approachability. A one-way repeated measures ANOVA revealed that Dog 1 (hanging ears, saber tail) and Dog 3 (hanging ears, docked tail) were rated as significantly safer to approach than Dog 2 (prick ears, saber tail) and Dog 4 (prick ears, docked tail). Multiple linear regression analyses revealed that childhood ownership, attitudes about dogs and fear of dogs were all significant predictors of perceived approachability. These findings have potential implications for dog bite prevention education. Participants' distinctions between the dogs raise important questions about whether people may misinterpret approachability based merely on ear or tail type. For example, if dogs with hanging ears are believed to be safer to approach, and if this belief supersedes recognition of signs of aggression, it may lead to risky interactions between humans and dogs.

## EYE WITNESS ACCURACY AND CONFIDENCE — IT'S ALL ABOUT THE GUN

Jessica Singer  
Faculty Research Advisors: Dr. Zachary Wilcox and Dr. Matthew Zagumny

The purpose of this research was to test the accuracy of eyewitness testimonies while introducing distracting items. Participants viewed one of six videos, each involving a different weapon and length of time the weapon was visible. The study utilized a 3(weapon) x 2 (weapon presence) x 2(criminal presence) completely between design. Two-hundred participants were randomly assigned to a video of a simulated robbery where the criminal is holding a knife, gun, or banana. A factorial ANOVA was conducted on memory confidence on a scale of 0-80. There was a significant main effect for weapon  $F(2,194)=4.48$ ,  $MSe=28.34$ ,  $p<.001$ . Participants who viewed a video including a gun were significantly more confident ( $M=45.45$ ) than those who viewed a video including a knife ( $M=43.24$ ),  $t(194)=2.69$ ,  $p<.05$  as well as those who viewed a video including a banana ( $M=42.87$ ),  $t(194)=2.69$ ,  $p<.05$ . Additionally, participants who viewed a video including a gun were significantly more accurate identifying the perpetrator in mug shots and choosing when he was not present in the mug shots ( $M=0.92$ ) than those who viewed a video including a knife ( $M=0.50$ ),  $t(194)=$ ,  $p<.05$ .  $F(2,194)=3.90$ ,  $MSe=.80$ ,  $p<.001$ . The results are interesting because participants were more confident in their memory of the event when a gun was present, even when they were not more accurate. One possible explanation is that a gun increases the emotional response of witnesses, resulting in greater confidence. Future research should examine the underlying processes that result in greater confidence but not accuracy, since there are serious legal implications for eyewitness testimony.

## PERFORMANCE ORIENTED SCHOOLS AND TEACHER BURNOUT: ROLE OF INDIVIDUAL TEACHER CHARACTERISTICS

Brittany Stephens  
Faculty Research Advisor: Dr. Zachary Wilcox

Federal and state governments in the United States have been emphasizing student performance through changes in educational laws, culminating with the No Child Left Behind Act in 2002. This emphasis on student performance may account for the increase in teacher stress, and if this stress is not coped with adequately, teacher burnout may occur. Predictor variables of teacher burnout were explored using 308 participants (53 male and 255 female). The participants in the study were elementary, middle, and high school teachers from East and Middle Tennessee. Participants were asked to complete a series of surveys that measured teacher burnout (emotional exhaustion, depersonalization, and reduced personal accomplishment), obsessive passion (internalizing one's career as one's identity), teacher self-efficacy (belief of what one can do successfully), and performance oriented school goal structure (stressing student competition when it comes to grades and intellectual ability). A multiple regression analysis revealed that obsessive passion, teacher self-efficacy, and sex of the teacher were significant predictors of teacher burnout. Interestingly, male teachers reported greater burnout than female teachers. Future researchers should continue exploring factors related to teacher burnout, as well as teacher well-being. Perhaps interventions can thus be developed to improve quality of life for teachers that will have a positive impact on the level of student achievement.

## USE OF SELF DETERMINATION THEORY NEEDS TO PREDICT MOOD DURING PHYSICAL EXERCISE

Josh Waddell  
Faculty Research Advisor: Dr. Zachary Wilcox

Previous research has shown that physical exercise does have a positive effect on both negative and positive moods. The goal of this research is to find what type of exercise has a significantly greater positive affect on both positive and negative moods. In addition, a need scale based on the self-determination theory will be used to find what needs are being met during the physical exercise routine. Participants will participate in either a weight-lifting routine, individual cardiovascular routine, or a cardiovascular class. The routine will be done just as they usually do on any day they come to the gym. The data will be calculated using a Multiple Regression analysis. The goal of this research is to identify which exercises and specific needs are the significant predictors that effect moods during physical exercise.

## EFFECTS ON THE PERCEPTION OF VICTIMS IN PSYCHOLOGICAL ABUSE SITUATIONS

Whitney Wells and Dr. Christopher Burgin  
Faculty Research Advisor: Dr. Christopher Burgin

Domestic violence is an epidemic that reaches across cultures and class lines. Statistics are plentiful on physical domestic abuse but statistics on women affected by non-physical domestic abuse are almost impossible to find and substantiate due to low reporting on the part of victim. Non-physical abuse may not cause visible damage; however it has a lasting impact on both the intended victim and unintended victims such as children. Psychological abuse can lead to a myriad of problems. This study focused on how belief in a just world and ambivalent sexism influence views of the victim and the perpetrator in psychological abuse. This research studied the impact of belief in a just world, hostile sexism, and benevolent sexism on a subject's view of selected psychological and nonphysical forms of domestic abuse. Participants age 18 to 73 of both sexes were solicited through social media. Results found two main effects. Participants who scored highly on the hostile sexism scale were more likely to blame the victim in the scenario as opposed to those who scored highly on benevolent sexism, belief in a just world, or did not score highly on any of the scales. The second of the main effects found that those participants were more likely to blame the victim and defend the perpetrator when the scenario gave no cause for the psychological abuse than the scenarios where reasons were given for the cause of the psychological abuse (family stress, weight gain, job stress, jealousy). There was also an interaction observed.

## CURRICULUM AND INSTRUCTION GRADUATE STUDENTS

### PREDICTIVE FACTORS OF SUICIDE IDEATION AND SUICIDE PLANNING AMONG U.S. ADOLESCENTS

Kimberly R. Hale and Rufaro A. Chitiyo  
Faculty Research Advisor: Dr. George Chitiyo

Literature suggests that systematic screening to identify students at risk for suicidal behaviors is an important component of prevention efforts (Gutierrez, Watkins, & Collura, 2004). The purpose of this descriptive correlational study was to examine predictors of suicide ideation and suicide planning among US adolescents by completing the 2009 Youth Risk Behavior Survey (YRBS). The YRBS is based on a nationally representative sample of youths surveyed on a variety of issues including drug use, sexual

and health behaviors, among others. The sample consisted of approximately 16, 200 adolescents. The predictors included various measures of drug use/abuse, bullying, and hopelessness. The dependent measures were suicide planning and suicide ideation. Binary logistic regression was used for analysis, owing to the dichotomous nature of the dependent variables. Findings of the study indicated feelings of hopelessness and bullying as the primary predictors of suicide ideation and planning. The results suggest that screenings that assess feelings of hopelessness and bullying should be an integral component of identifying youth at risk for both suicide ideation and planning.

### ENGINEERING EDUCATION - DEVELOPMENT OF RENAISSANCE ENGINEERS

Lacy Loggins  
Faculty Research Advisor: Dr. Pedro E. Arce  
Collaborator: Dr. Pedro E. Arce

This research is a qualitative study that is focused on one of the key aspects of the High Performance Learning Environments (Hi-PeLE) as a tool for enhancing innovation in the development of renaissance engineers according to the USA National Academy of Engineering (NAE) 2020 Model. One of the key motivations is to empower students to take responsibility for their own learning instead of being "spoon-fed" with information done in the traditional engineering education environment. This is challenging because most engineering classes are taught using traditional methodologies, for example: lectures, quizzes, homework, and exams with little or no collaboration among peers. They also have little or lack opportunities for engagement in learning and fostering skills for innovative approaches. In this research, Hi-PeLE was applied to a junior level course in the Chemical Engineering program at Tennessee Technological University (TTU).

### WHAT PREDICTS MATH UTILITY PERCEPTIONS AMONG HIGH SCHOOL FRESHMEN?

Twanelle Majors and Jennifer Meadows  
Faculty Research Advisor: Dr. George Chitiyo

The purpose of this study was to explore the construct of math utility among high school students using data from the High School Longitudinal Study of 2009, conducted by the National Center for Education Statistics. The construct of math utility, measured from self-reported variables of students' perceptions on the utility of math, and generated using principal components factor analysis, was significantly negatively related with students' actual test performance on a criterion-referenced mathematics cognitive test. The Cronbach's alpha coefficient of reliability (.65) showed that the utility construct was reliably measured. We thus used a multilevel regression analysis to predict math utility from a

set of variables including students' math identity and math self-efficacy constructs, teacher reported variables including their own perceptions of self-efficacy, their emphases on certain aspects of math such as problem solving, business/industry applications and preparation for future math study. Among other findings, the students' self-efficacy and math identity were significant predictors as well as the teachers' emphasis on real world applications of mathematics. Using a stepwise regression showed that the model significantly improved by including math achievement as an additional predictor (the R-Squared changed from .147 to .157).

## FUNDING TRENDS OF NSF INFORMAL SETTING (AISL) STEM LEARNING GRANTS

Twanelle Majors, Jennifer Meadows, and Laura Luna  
 Faculty Research Advisor: Dr. George Chitiyo  
 Collaborator: Dr. Hyuksoo Kwon (Kongju National University, South Korea)

Over the last few years, K-12 STEM education has attracted significant attention at the policy-making level. This is partly due to the societal emphasis on implementation of formal STEM education. Some of the concerns in this area of STEM education relate to the insufficient preparation of K-12 STEM teachers and low academic achievement of K-12 students toward STEM subjects. STEM researchers and practitioners have suggested that informal STEM learning opportunities are as important as formal K-12 STEM learning. The goal of this study was to investigate contemporary research trends and priorities of STEM education, especially in informal settings. We reviewed abstracts from relevant studies investigating K-12 STEM education in informal settings in order to identify STEM education research studies which were funded. The analysis sought to obtain data such as project goals (objectives), concentrated disciplines, outreach institutes, target audiences (grade, gender, race, etc.), and their expected implementation strategies for all the abstracts of NSF (National Science Foundation) funded projects. Targets for these analyses were limited to searchable research papers (Advancing Informal STEM Learning (AISL) under the NSF DRL division: Research on learning in formal and informal setting. The findings of this study can be used as an outline for designing K-12 STEM outreach related research and projects for which funding is sought.

## MOTIVATING MINDS: HOW BOOK SELECTION IN PRESCHOOL CLASSROOMS AFFECTS READING MOTIVATION

Amber Spears and Rebekah Marcum  
 Faculty Research Advisor: Dr. Deborah Setliff

The purpose of this research will be to describe and compare the reading behaviors used by preschool children during

free reading time. Children who are read to at an early age are more likely to have increased vocabulary, early reading performance, and later success in school. Approximately twenty children from a local preschool will be observed during reading center time over the course of two weeks. Observational notes and data will reveal the types of books that children choose most often during independent book reading time. We will be examining time spent with each book, the genres of books chosen most frequently and comparing these differences across age and gender. Results from this pilot study will drive future research endeavors.

## CURRICULUM AND INSTRUCTION UNDERGRADUATE STUDENT

### PLEASURE PACKS A PUNCH

Emily Thompson and Amanda Ellis  
 Faculty Research Advisor: Dr. Julie Baker

Pleasure reading: The two words often don't meet in adolescent vocabulary and they most certainly don't come together at school. High stakes testing and teacher evaluation systems don't take into consideration whether students enjoy reading. Results may be surprising if students are given opportunity, access, and choice to read what they want in school. This interpretive study explored adolescent pleasure reading by taking a variety of student-chosen books into classrooms and providing time to read in class. Adolescent interviews supplied insight into their experiences of reading for fun at school. Teacher interviews, adolescent journals, book projects, and class observations were included as data collection. The importance of adolescent voice was illustrated in preliminary results indicating piqued student interest in reading and more open conversations about reading as well as learning in the classroom. Adolescents also reveal more about motivation and engagement, as well as common school practices that discourage reading.

## CHEMICAL ENGINEERING GRADUATE STUDENTS

### CONCENTRATION PROFILE OF OSCILLATION ANNEALED PCBM IN P3HT FILMS

Preejith Ambuken and Dr. Holly Stretz  
 Faculty Research Advisor: Dr. Holly Stretz

Gas expanded liquid (GXL) deposition technology has previously been shown to anneal systems of gold nanoparticles in a monolayer on a surface. The current

work will demonstrate the ability to anneal (equilibrate) fullerene or 1-(3-methyloxycarbonyl) propyl (1-phenyl [6,6] C61 (PCBM) nanoparticle morphology in a 3-D film of finite thickness composed of polymeric Poly(3-hexylthiophene) (P3HT). This P3HT/PCBM thin film layer is used as an active layer in organophotovoltaic cells. Good dispersion of PCBM in P3HT results in improved performance and efficiency of the device. PCBM has been shown to adopt a non-uniform concentration profile. Annealing of the as-cast morphology is often required to realize this morphology and improve the device performance. A novel method is being developed to solvent-anneal the films, wherein solvent vapor exposure is supplemented by oscillations in solubility using the gas expanded liquid (GXL) process. The annealing process will be carried out in a specifically designed high pressure CO<sub>2</sub> reactor. X-ray Diffraction and contact angle testing is used to characterize the P3HT/PCBM samples that are pressure annealed under different conditions.

### MORPHOLOGICAL AND THERMAL CHARACTERIZATION OF TPU AND TPU/PA11 NANOCOMPOSITES

Preejith Ambuken and Dr. Holly Stretz  
Faculty Research Advisor: Dr. Holly Stretz  
Collaborators: Dr. Joseph Koo (The University of Texas at Austin) and Derek Wong (The University of Texas at Arlington)

In this study thermoplastic polyurethane (TPU) and thermoplastic polyurethane/polyamide11 (TPU/PA11) nanocomposite blends were prepared via melt compounding by incorporating Cloisite30B (CI30B) and multi walled nano tubes (MWNT) as nanoparticles. Morphological characterization of all the samples were done using x-ray diffraction (XRD) while thermal characterization was carried out using Differential Scanning Calorimetry (DSC), Dynamic Mechanical Analyzer (DMA) and high temperature x-ray diffraction (HT-XRD). From xrd results, it was found that CI30B platelets completely lost registry with each other and were able to obtain intercalated structure by melt compounding. DSC and HT-XRD revealed the crystallization pattern of TPU/PA11 nanocomposite blends. DMA results indicated that addition of PA11 also resulted in improved performance of depression in storage modulus which takes place due to the melting of hard segments of TPU. Visual observation of char obtained from DMA also revealed information of char structure with the characteristic patterns obtained by the addition of specific nanoparticle.

### CHEMICAL DEGRADATION OF XANTHATE BY PULSE CORONA DISCHARGES

Katherine Cerda and Dr. Pedro E. Arce  
Faculty Research Advisor: Dr. Pedro E. Arce

This work is focused on the degradation of xanthates waste used in flotation process from copper mining companies, which are organosulfur compound useful in the extraction of certain ores, in this case sulfide ore. These wastes are often deposited on tailings -pile in areas surrounding the mine site, and sometimes they drain-down. For this reason, it will be useful to degrade them instead of being deposited. A very promising high oxidation technique based on electrical discharges will be used as the key method for the degradation of xanthate in this research project. This presentation will overview both oxidation technique as well as the plan to conduct preliminary studies of feasibility for the degradation of xanthate in aqueous solution.

### QUANTITATIVE CHARACTERIZATION OF FLY ASHES: APPLICATION IN THE GEOPOLYMER CEMENT

Ojas Chaudhari  
Faculty Research Advisor: Dr. Joseph J. Biernacki

Portland cement, the basic ingredient in concrete, is the most commonly used construction material in the world. However, portland cement production results in the generation of greenhouse gases from both energy consumption and chemical changes associated with the production process. In general, production of one ton of portland cement results in approximately one ton of the greenhouse gas, CO<sub>2</sub>, released into the atmosphere. In an effort to reduce our dependence on traditional portland cement-based concrete, ongoing research is concentrating on development of new low environmental impact alternative cements. Geopolymer cement concrete is one recently developed alternative. Geopolymer cement concrete uses different raw materials and different production processes than portland cement, which enable a five to six times reduction in greenhouse gas emissions. The process for geopolymer production includes mixing an anhydrous aluminosilicate material with an alkaline solution such as sodium or potassium hydroxide. The industrial waste fly ash can be used as a potential source of the aluminosilicate materials required in geopolymer cement production. The mineralogy of the fly ashes, including the proportions of crystalline phases (quartz, mullite, hematite, magnetite etc.) and amorphous phases directly affects the rate of the geopolymerization reaction. Therefore, quantitative characterization of crystalline and amorphous phases in the fly ash is an essential requirement for the accurate study of the geopolymerization reaction. In this research, the proportion of amorphous (glassy) material in one low and one high LOI fly ash has been evaluated by X-ray powder diffraction (XRD) using the Rietveld quantitative phase analysis method. Two different, X-ray processing modes were investigated including parallel beam and Bragg-Brentano mode. Furthermore, two different

internal standards (corundum and rutile) were used. A good estimate of the percentage of amorphous phases present in the low and high LOI fly ashes was made using the Rietveld XRD method. The results of quantitative XRD analysis of low LOI fly ashes were found to be consistent with published data for fly ash samples. The obtained results will be helpful to understand reactive (amorphous) components of the fly ashes.

### ELECTRO-ASSISTED SEPARATION OF PARTICLES: AN EFFICIENT STOCHASTIC-BASED APPROACH

Parvin Golbayani, Dr. Motoya Machida, and Dr. Pedro E. Arce  
Faculty Research Advisors: Dr. Pedro E. Arce and Dr. Robby Sanders

Separation of particles by electrical-based methods has been the subject of numerous studies 1, 2 and a number of techniques have been developed 3. The key interest arises from the large volume of business generated by the field. Examples include pharmaceutical 4, clinical diagnostics 5 and environmental proteomics 6 among others. The focus of this research is on the use of stochastic-based approach to obtain effective mobility and effective diffusivity coefficients. This, to the best of our knowledge, would be the first effort to determine the time of separation of two similar particles under an applied electrical field, i.e. "Biased Brownian Motion of Polyelectrolyte under an Applied Electrical Field". The analysis involves the solution of the equation of motion of a Brownian particle by using a Langevin equation 9. In this research, we have been studied separation time of Lysozyme (LYZ, MW:14.4 KDa) and Cytochrome c (CYC, MW: 11.7 KDa) in presence of both constant and linear electrical field in stationary fluid. Moreover, effective mobility and effective diffusivity were obtained in Poiseuille flow by solving nonlinear stochastic differential equation. Result of this investigation is consistent with Taylor-Aris dispersion. Results will be useful pieces of information at the device level and illustrated with parameters beneficial for practitioners. In summary, this project offers a very efficient path to obtain vital information to guide both experiments and new research relevant to both environmental proteomics and clinical diagnostics.

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### MULTI-IONIC CONTINUUM-BASED ADVANCED SINGLE PARTICLE MODEL FOR C3S/ALITE HYDRATION

Manohar Gottapu and Dr. Joseph J. Biernacki  
Faculty Research Advisor: Dr. Joseph J. Biernacki

Alite (impure mineral monoclinic tricalcium silicate (C3S(m))), the major constituent of ordinary portland cement (OPC), when mixed with water, rapidly dissolves and reacts to form a cementitious hydrated porous product (calcium silicate hydrate (C-S-H)) and a non-cementitious crystalline byproduct (calcium hydroxide (CH)) via coupled reactions of dissolution and precipitation. Referred to as hydration, this complex process effects the most important application oriented characteristics of concrete including workability, set time, the rate of heat evolution, and the ultimate strength and the durability. Recent modeling strategy based on an advanced single particle model illustrated the utility of continuum-based models for the elucidation of such complex hydration processes. The present work further extends the approach to a robust modeling platform considering rigorous multi-ionic transport, non-linear equilibrium (reversible) reaction kinetics, particle ensemble features such as neighboring particle proximity and volume filling effects and the implementation of an Avramian representative volume concept. The model also includes diverse mechanistic characteristics: nucleation and growth, surface area reduction, and two-step densification. Such a multi-constrained model is not only able to quantitatively capture the observed calorimetric hydration behavior, but also, predicts the corresponding pore solution evolutions.

### APPLICATION OF PULSED CORONA DISCHARGES (PCD) IN WATER TREATMENT

Negin Koutahzadeh and Dr. Pedro E. Arce  
Faculty Research Advisor: Dr. Pedro E. Arce

A corona discharge is an ionic and electronic emission from a high voltage corona, characterized by the formation and flow of positive and negative ions and electrons in an electric field between two or more electrodes. The pulsed corona discharge causes the formation of hydroxyl radicals, hydrogen peroxide, and aqueous electrons. Several other species such as  $\cdot\text{OH}$ ,  $\cdot\text{O}$ ,  $\text{O}_3$  are also important reactants. These species are important to treat water. For example Hydroxyl radicals directly attack organic compounds leading to the oxidation of these compounds. Grymonpré et al (2001), investigated the effect of Pulsed corona discharges at breaking down Phenol in aqueous solutions in an isothermal batch reactor and in a semi-batch reactor with the continuous addition of oxygen and they found that Pulsed Corona Discharges (PCD) is effective for degradation

of phenol in aqueous solution. The PCD technique involves a complex set of physical and chemical reactions such as voltage level and frequency of the pulsed corona system, solution composition, pH, molecules initial concentrations, DOC (Dissolved Organic Carbon) values as a function of treatment time "arc time" and conductivity. In our study we investigated the physical and chemical reactions that occur in PCD and their critical roles in water treatment. Keywords: Pulsed Corona Discharges (PCD), physical and chemical reactions, Streamer discharges, Spark discharges, radicals.

### DETERMINATION OF NORMAL AND MUTANT ALPHA-1-ANTITRYPSIN INHIBITION ACTIVITIES

Bryan Materi  
Faculty Research Advisor: Dr. Robby Sanders

Alpha-1 antitrypsin (AAT) is the most prevalent serine protease inhibitor in the human body. It protects connective tissue components (particularly elastin) from degradation by elastase (a product of certain white blood cells) and helps guard against the damaging effects of cigarette smoke and other toxins in the lungs. Approximately 100,000 people in the United States have been diagnosed with an inherited condition in which AAT is not properly made. As such, these people are considered to have AAT deficiency and are predisposed to early onset emphysema, liver damage, and other health conditions. It is estimated that 3.4 million people worldwide actually have this disease that are related to this condition. Another 117 million people are carriers. With these estimates, improved therapeutics and diagnostics are needed for this condition. Thus, this research is focused on the determination of "activities" of normal and mutated forms of AAT. Towards this end, fibroblasts will be transfected with plasmid DNA containing each of three versions of the AAT gene. The expressed protein will be collected and assayed for activity by measuring the capacity of the protein to inhibit elastase. Such efforts are part of a long term goal to develop a diagnostic device for AAT deficiency.

### MODELING FIBER PACKED-REACTOR UNDER LAMINAR REGIME

Chinyere P. Mbachu  
Faculty Research Advisor: Dr. Pedro E. Arce  
Collaborators: Dr. Holly Stretz and Dr. Ahmed Elsayy

Modeling of novel fiber-packed reactors for the production of chemicals, including biodiesel, nanoparticles, and others is an important and relevant aspect in order to help or improve scaling and designing aspects of these reactors. These packed-bed fiber reactors take advantage of the unique features of the fibers that provide an enormous area

of contact (for two phases) without the need of mixing. The research approach focuses on developing a transport model (under laminar regime) with the associated kinetics to study of dynamic of convective-diffusion taking place inside the novel fiber-packed reactors for the production of chemicals such as biodiesel, nanoparticles, etc. A continuum-based approach with proper assumptions will produce a "single-phase" model, first, to predict the conversion. After an understanding has been achieved, more complex models, i.e. introducing the two phases will be developed. Several limiting cases of both kinetics and transport will be studied in order to gain understanding of the system behavior. Both analytical and computational-based approaches will be used in order to illustrate the version of the model predictions.

### ELECTROSTATIC POTENTIAL IN ANNULAR GEOMETRY

Abbas Motamedilamouki, Dr. Pedro E. Arce, and Dr. Robby Sanders  
Faculty Research Advisors: Dr. Pedro E. Arce, and Dr. Robby Sanders

Flow through an annular geometry has many applications in chemical, environmental, mechanical and biomedical engineering areas [1]. In order to model the electrokinetic transport, here a systematic investigation of the electrostatic potential distribution in an annular geometry is presented. The analytical solutions for the electric potential profile in the annulus are obtained by solving the 2D Poisson-Boltzmann equation with both long channel and Debye-Huckel approximations. This result is in preparation to the derivation of the electrohydrodynamic velocity profile. The ultimate goal of this research is to understand the role of capillary geometry in determining biomolecular motion inside capillary domains that are relevant for drug delivery, separation, or nutrient transport in tissue scaffolds. As a result of this investigation, one can assess the behavior of the electrostatic potential inside of annular channel. Three key parameters have been identified to describe the electrostatic potential behavior: the angle ( $\alpha$ ), ratio of up wall potential to the linear combination of both wall potentials,  $R$ , which handles the symmetrical/non-symmetrical aspects of the electrostatic potential, and the ratio of the width to the length ( $\Gamma$ ) that controls the "shape" of the channel section. Results of this study are illustrated by using a series of portraits that capture the key behaviors of the electrostatic potential with respect to the three parameters described above.

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## IN SILICO SCREENING FOR NOVEL INHIBITORS OF HUMAN NEUTROPHIL ELASTASE

Christian Nguyen

Faculty Research Advisor: Dr. Robby Sanders

Collaborator: Dr. Jens Meiler (Vanderbilt University)

The discovery of drug like compounds that inhibit Human Neutrophil Elastase (HNE) could lead to therapeutic products for treating alpha-1-antitrypsin deficiency (A1AD), an inherited condition that predisposes those affected to early onset emphysema. Efforts have been made towards the development of therapeutic low molecular weight inhibitors for HNE, but as of now, no such compound has been approved for treating A1AD. Towards this end, a collaborative, inter-institutional team has pursued a therapeutic drug discovery methodology consisting of a novel integrated computational approach that incorporates virtual high-throughput screening (HTS), clustering, and protein-ligand docking. Artificial neural networks and decision trees machine learning methods have been applied to produce Quantitative Structure Activity Relationship (QSAR) models that predict the biological affinity of compounds with HNE based on their IC50 values. The QSAR models were used for virtual HTS, and the top 0.05% of compounds predicted to have the highest binding affinity was selected for a clustering analysis. The clustering analysis compared the atom type and structure of the predicted compounds with known active inhibitors. From virtual HTS and clustering analysis, 20 compounds were selected from a chemical library of 200,000 such that the greatest difference in structure and atom type was identified to insure the highest probability of finding new chemotypes. These compounds were virtually docked into the HNE structure to prioritize them based on the predicted binding affinity and docked conformation. Experimental studies with these 20 compounds are being conducted to validate model predictions and document the potential of these compounds to inhibit HNE.

## VOLUME AVERAGING APPROACH FOR SCALING A POROUS ELECTRODE IN ELECTROCHEMICAL SYSTEMS

Njideka H. Okoye

Faculty Research Advisor: Dr. Pedro E. Arce

This research focuses in understanding further the species mass transport and electrochemical reactions in porous electrode systems. These systems are important in environmental and industrial applications e.g. fuel cell electrode, batteries. The Volume Averaging Theorem (proposed by Whitaker and others) will be the central tool used to derive electrode-pore scale and spatially-averaged equations valid for the electrode-domain level. In

understanding this concept, the species mass conservation equation will be up-scaled for both cases, i.e. with and without electrochemical reaction and also in the presence of electromigration. A closure level equation will be incorporated into the scaled-up model in order to know the denominating terms affecting electrochemical processes on the porous electrode domain. Limiting cases will also be analyzed and compared with results from the literature that are currently available but obtained by using other approaches.

## SUBZERO FUEL CELL PERFORMANCE ENHANCEMENT VIA CATALYST LAYER ADDITIVES

Antonio Pistono and Dr. Cynthia Rice

Faculty Research Advisor: Dr. Cynthia Rice

Polymer electrolyte fuel cells are the de facto replacement for internal combustion engines for automotive applications as the auto industry moves to greener fuel sources. Since the product of a hydrogen-air fuel cell, pure water, can freeze within the macro-homogeneous porous catalyst-layer matrix during subzero operation, one of the most challenging issues is the ability for the fuel cell to self-heat. The exothermic oxygen reduction reacts to above 0C, therefore allowing for the product water and ice removal through melting and evaporation.

The time for the cell to heat due to the exothermic reaction is generally balanced with the accumulation of product ice in the catalyst layer eventually causing failure due to blockage of the reactant gasses to the catalyst surface. Testing using isothermal and applying constant current conditions was used to determine how much water or ice the catalyst layer can store at a given current before the cell fails. To this end, additives were incorporated to the catalyst layer to enhance the water storage capability of the fuel cell by increasing 1) the open pore volume and 2) the acidity of the matrix material. Electrochemical impedance spectroscopy was used to evaluate the state of the catalyst layer (at subzero conditions) before and after to determine isothermal constant current testing, to probe water content and determine the diffusional resistance. Increasing the acidity allowed the fuel cell to store more water with high initial water content. Increasing the open pore volume increased performance under high load operation.

## INVESTIGATION OF HUMIC ACID AGGREGATION BY ZETA POTENTIAL AND DYNAMIC LIGHT SCATTERING

Milad Rabbani Esfahani, Dr. Holly Stretz, and

Dr. Martha J. M. Wells

Faculty Research Advisors: Dr. Holly Stretz and

Dr. Martha J. M. Wells

While natural organic matter and specifically humic acids (HA) have been studied extensively, the aggregation of these materials in solution is not well understood. In this study, the effects of time, concentration, and filtration (through a 0.45 micron Millipore filter) were examined by monitoring changes in zeta potential and dynamic light scattering. The effects of the concentration were studied at 2, 5, 8, 45, 100, 250, and 500 ppm. At lower concentrations of HA, higher variation of aggregation size was observed compared to higher concentrations. Zeta potential decreased and became more negative as concentration increased. The data generated in this research will be compared with other studies of HA aggregation.

## PNIPAM MONODISPERSION FOR USE IN HYDROGELS

Alex Sherrill and Dr. Holly Stretz  
Faculty Research Advisors: Dr. Holly Stretz and Dr. Pedro E. Arce

This research focuses on creating poly (N-isopropyl acrylamide) (PNIPAM) microparticles of a uniform size using a novel fiber film reactor. A secondary focus will be to attempt through variation of reactor parameters or composition to vary the lower critical solution temperature (LCST) of the microparticles. These microparticles, which are thermoresponsive, can be embedded in a hydrogel and create a gel with a tunable porosity for protein separation. When heated, the microparticles undergo a LCST phase transition and shrink in volume by a measureable amount, allowing the size of the pores they leave behind to be known. With a monodisperse microparticle size, gels can be created with more consistent structure, thus allowing for better control of protein separation. Batch microparticles have been created, and the particle size distribution has been determined using Dynamic Light Scattering. The batch microparticles have been shown to have an LCST. Further, the fluid dynamics of the fiber reactor have been characterized.

## DEVELOPING TOMORROW'S SUSTAINABLE INFRASTRUCTURE USING COMPUTER AIDED MOLECULAR DESIGN

Natalia Shlonimskaya  
Faculty Research Advisor: Dr. Joseph J. Biernacki  
Collaborators: Hamed Kayello (University of Akron) and Dr. Donald Visco (University of Akron)

Repairing our concrete infrastructure requires new concrete materials that are sustainable and perform better than the materials preceding them. Cracking of concrete is a major problem. Shrinkage caused by water's high surface tension

is among the primary cause of cracking. Surprisingly, the tension in the surface of water is so great that it can actually produce enough force to pull the concrete inward and make it shrink. Since some organic chemicals can reduce the surface tension of the water, it should be possible to design custom compound that have a high propensity to lower surface tension and thus inhibit shrinkage of concrete. A unique aspect of this work is applying, for the first time, a process called Computer Aided Molecular Design (CAMD). CAMD uses information about how known substances behave, encodes their molecular structure and relates it to their performance, and then uses that information to predict new molecules with expected improved performance. A number of potential new shrinkage reducing structures have been designed using this CAMD approach. This research focuses on testing of the new CAMD designed molecules and improving the model predictions.

## MODELING ELECTROKINETIC-SOIL CLEANING BY SPATIAL AVERAGING

Rocio Tijaro-Rojas and Dr. Pedro E. Arce  
Faculty Research Advisor: Dr. Pedro E. Arce

To predict the transport of ionic species into anisotropic porous media, such as soils, when an external electric potential is applied, this research will use a multi-scale modeling approach. A minimum of key simplifications will be used, in order to capture the fundamental system behavior in model soils that mimic actual ones. Geometry of the control volume, medium properties, and intensity of electric potential constitute important variables to be considered. Since, the mass transport of the ionic species in soils takes place in a domain that displays different scales (molecular, microscopic, macroscopic and mesoscale), a multi-dimensional (spatial) averaging approach will be applied. Once, the spatial-averaged model become available, computational approaches will be used to illustrate the behavior of fundamental aspects. As a complementary part of this research, an experimental approach is being developed (in collaboration with an undergraduate student) to guide and validate the predicted results.

## STUDY OF ELECTRODEPOSITED NI-CO ALLOY COATING ON FERRITIC STAINLESS STEEL

Linzhu Zhang  
Faculty Research Advisor: Dr. Ying Zhang

Ferritic stainless steels have become the standard material for SOFC interconnect applications due to their CTE match with ceramics, excellent formability and low cost. Nevertheless, under SOFC operating conditions (high-

temperature, wet and O<sub>2</sub>), ferritic stainless steels suffer from several shortcomings. Numerous coatings, surface treatments and alloy bulk composition modifications and developments have been considered as potential remedies in order to overcome these issues. Spinel coatings have attracted significant attention recently. Because spinels have good electronic conductors and show excellent CTE match with the ferritic stainless substrate and other cell components. Spinel coatings have also shown excellent capability for absorbing Cr. Recently, electrodeposition of metals followed by heat treatment/oxidation has been considered as a novel technique for spinel coating. The research investigated electroplating Ni-Co alloy on ferritic stainless steels and followed by heat treatment in air at 800°C in order to form a (Ni,Co)<sub>3</sub>O<sub>4</sub> spinel coating on the surface of the interconnect. The effects of pH and temperature of plating solution as well as the cathode current density on the quality of Ni-Co alloy coatings were studied. The area specific resistance (ASR) of the oxide scale was measured. Morphologies of the coating and its oxide scale were observed using SEM, EDS and their phase structures were identified by XRD. Furthermore, Ni-Co-CeO<sub>2</sub> composite coating were electrodeposited on ferritic stainless steels in order to improve the properties of the coatings on the aspect of decrease the thickness of the oxide scale and the rate of oxidation.

## CHEMICAL ENGINEERING UNDERGRADUATE STUDENTS

### TARGETED GENE DELIVERY TO THE LUNGS

Chelsea Creutz and Dr. Robby Sanders  
Faculty Research Advisor: Dr. Robby Sanders

There are numerous genetic mutations that lead to inherited diseases of the lungs. For many of these conditions, therapeutic strategies are inadequate because they only treat symptoms of the disease and not the underlying problem. Gene therapy is one approach to correct faulty genes responsible for the disease development. While still under development, this approach may prove beneficial for the treatment of various pulmonary diseases such as cystic fibrosis, alpha-1 antitrypsin deficiency, primary pulmonary hypertension, lung cancer, and asthma. Through gene therapy, vectors with the normal gene are delivered directly or indirectly to the target site (cell). The vectors are either viral or non-viral based. To combat potential viral vector toxicity, there has been a vast growth of research into non-viral vectors (for example, liposomes, dendrimers, polyethyleneimines, etc.) and modes of delivery. Inhalation therapy delivered as aerosols is one application of the non-viral vector method. Developments in aerosol delivery systems have resulted in major advances toward potential applications for various diseases of the lung. Near

instantaneous and direct transmission to the lungs makes aerosols ideal to avoid potential harmful side effects that often occur following systemic (oral, intravenous, etc.) delivery. Furthermore, the lungs are a great candidate for these drug-laden aerosols because of their large surface area which is ideal for the movement of drug into the tissue. This research explores these advances in gene delivery affecting the lungs.

### SOLVENT ANNEALING OF P3HT FOR CRYSTALLINITY CONTROL IN ORGANIC PHOTOVOLTAICS

Brian Daniels, Preejith Ambuken, and Dr. Holly Stretz  
Faculty Research Advisor: Dr. Holly Stretz

The application for this research is to stabilize and control the dispersion of nanoparticles for use in organophotovoltaic cells. To do this, it is necessary to control the crystallinity of the photoactive polymer (P3HT). The research question then becomes can we remove crystals from a spin-coated thin film of P3HT post-deposition by solvent annealing and subsequently regrow them? Solvent annealing is commonly used to grow crystals; but the mechanism is not well documented. The current goal of this project is to examine the effect of time on the solvent annealing process. This is achieved by building a system in which solvent vapor anneals the P3HT while x-ray diffraction (XRD) is performed in situ. This allows real time analysis of both annealing and the drying after the solvent vapors have been removed. The real time data will allow a greater understanding of the mechanism by which the crystals form or melt. Early data has shown a slight shift in the angle of the XRD peak. This result is surprising and may indicate a change in the crystal structure depending on how the sample is annealed.

### QUARTZ CRYSTAL MICROBALANCE TO QUANTIFY FUEL CELL CATHODE CATALYST LOSS (AUTOMOTIVE)

Brandon Davis and Dr. Cynthia Rice  
Faculty Research Advisors: Dr. Patrick Urchaga and  
Dr. Cynthia Rice

A major deterrent to mass commercialization of polymer electrolyte membrane fuel cells for automotive applications is platinum (Pt) cathode catalyst degradation due to exposure to idle-to-peak power transient conditions. The purpose for quartz crystal microbalance is to study the loss of active electrochemical surface area (ECSA) on a Pt coated quartz crystal. Potential perturbations observed in automotive idle-to-peak power transients cause ECSA decreases, which is an undesired effect for performance

and cost. The results of this study are intended to aid in the progression of the sustainability of fuel cells, through mechanistic understanding. The experiments are run with a Pt coated quartz crystal cell in acidic electrolyte solutions of different molarities to emulate relative humidity cycling typically experienced during automotive operation. A potential is applied to the Pt on the crystal to induce oxide formation and subsequent reductions. The mass (lower sensitivity limit 0.4 ng/cm<sup>2</sup>) and current responses are acquired simultaneously. The findings show that the ECSA decreases with each successive experiment. The results are anticipated to result in new metallic catalyst combinations and operational constraints that will survive automotive applications. This will directly aid in the development of fuel cells that will last longer in our future vehicles.

### QUANTITATIVE ANALYSIS OF LIPOPOLYSACCHARIDE CONCENTRATIONS IN A MICROFLUIDIC DEVICE

Dominick DeChristofaro  
Faculty Research Advisor: Dr. Robby Sanders

Endotoxins (also known as LPS or lipopolysaccharides) are membrane-bound molecules that protect gram-negative bacteria and provide structural integrity to these ubiquitous microbes. As LPS is pyrogenic (i.e., causes fevers in humans), levels of endotoxin must be minimized in water-based solutions or other components that may be used in treating various health ailments. Limulus Amebocyte Lysate (LAL) is an aqueous extract of blood from the horseshoe crab used in assays to detect endotoxin concentration. There are several ways to detect endotoxin concentration with gel-clot, turbidimetric, and chromogenic-based LAL testing being the most popular within the pharmaceutical production and medical device industries. Such approaches utilize relatively large quantities of assay reagents (hundreds of microliters) and may require expertise in interpreting results (gel clot). We are proposing a new device that is hypothesized to enable quantitative results of gel-clot testing by correlating pressure and Endotoxin Units (EU) using a microfluidic device. By varying the number of EU, and correlating these to pressure, we hope to reduce cost, increase accuracy, and produce quicker LAL gel-clot test results. If effective, such technologies could be utilized in industry for enhanced screening of pharmaceutical compounds and medical devices prior to their use in treating various conditions.

### TECHNIQUES IN THE PREPARATION OF ADDITIVE ENHANCED MEMBRANES FOR PEM FUEL CELLS

Jeremy Douglas and Anthony Addington  
Faculty Research Advisor: Dr. Cynthia Rice

Hydrogen fuel cells are a potentially viable alternative power source. Improving proton conductivity increases the efficiency and practicality of hydrogen fuel cells. S-ZrO<sub>2</sub> is a superacid and is anticipated to enhance membrane conductivity due to enhanced acidity and proton availability. However, uniform through-plane distribution within a 25-50 μm thick membrane is problematic due to aggregation and segregation of the S-ZrO<sub>2</sub> (20nm) particles. Two methods for producing perfluorosulfonic acid (Nafion) S-ZrO<sub>2</sub> modified membranes are developed and ex-situ proton conductivity measurements are used to evaluate the membranes. A (i) spray method in which a dilute Nafion solution is sprayed onto a substrate and (ii) a drop casting method in which Nafion solution is recast onto a substrate was developed to produce baseline Nafion membranes. Membranes are tested by measuring conductivity at various temperatures and relative humidities. S-ZrO<sub>2</sub> additive membranes will be then prepared and tested. The spray method is expected to have more uniform distribution than the recast method.

### WATER UPTAKE ANALYSIS OF FUEL CELL MEMBRANES USING DIFFERENTIAL SCANNING CALORIMETRY

Adam Edwards and Kierna Mason  
Faculty Research Advisor: Dr. Cynthia Rice

Proton exchange membrane fuel cells (PEMFC) are a developing technology that has the potential to reduce society's reliance on fossil fuels. In automotive applications PEMFCs are regularly subjected to subzero temperatures. The freezing of water in the internal pore structures of the Nafion membrane has effects on the proton transport capabilities and water distribution of fuel cells. A fraction of water at subzero temperatures is known to remain in a non-frozen super-cooled state that contributes to redistribution of proton conduction. Differential scanning calorimetry (DSC) is used to analyze the amount and characteristics of water in Nafion and membrane catalyst layers that have been subjected to various relative humidities.

### BACTERIAL PROTEIN DETECTION

Melea Gilmore  
Faculty Research Advisor: Dr. Robby Sanders

Water is arguably the most important and valuable resource in the world. Without clean, fresh water, life as we know it would not exist. We as a society are aware of this. In fact, billions of dollars are poured into water testing and into treatment plants every year. My goal is to make that process more efficient and affordable. By understanding and measuring the types and quantities of enzymes that are secreted by bacteria and other microbes, we hypothesize that the types of microbes that may be in the water being

tested can be determined. The technique that I want to apply utilizes an agarose resin towards a novel detection methodology of various extracellular enzymes. This material can be purchased with substrates and placed into a plastic chromatography column then the liquid sample can be passed through the system. If the sample contains certain enzymes, these should act on the specific substrate and create a measurable signal. Over time, we hope to combine agarose resins with various substrates in the same column and determine whether a characteristic "signature" can be detected for the particular microbes that are present in the sample. Ultimately, we will create a portable microfluidic device that can process the extracellular enzymes and provide an immediate read-out of the microbes that are currently present in the water. By doing so, we will be able to enable a faster response to detect contaminants that might otherwise take weeks to find and years to contain.

### FAST PYROLYSIS OF BIOMASS PARTICLES

Jeff Glancy

Faculty Research Advisor: Dr. Joseph J. Biernacki

Biomass pyrolysis is being developed as an advanced bio-resource alternative to ethanol. Expectations are that pyrolysis generated oils (bio-crude) may soon provide large amounts of sustainable feedstock for producing fuels and chemicals and reduce our dependence on fossil resources. A microscale study of fast pyrolysis reactions is being conducted at TTU to develop a mechanistic understanding for focused product production and reactor design and optimization. The particles being studied are alfalfa stems milled into a flour and spray-dried to form nominally 300  $\mu\text{m}$  diameter spheres. A single particle is injected, along with an inert carrier gas, into a 1 mm ID quartz glass tube which is heated in a small oven to the desired test temperature. The particle is trapped inside the reactor and pyrolyzed. The pyrolysis gasses produced are sent to a FID (flame ionization detector) to determine the rate of pyrolysis. The preliminary data shows a good correlation between the particle volume and quantity of pyrolysis gas. The current detector being used, however, is not fast enough to capture accurate kinetic data. Research is currently being conducted to find a detector with faster response times. Additionally, a computer model of the reactor is being developed to predict reactor behavior and give insight into current pyrolysis data.

### UNDERSTANDING THE CYTOTOXICITY OF THE POLYAMIDOAMINE DENDRIMERS IN CELLS

Jerry Igiozee and Dr. Robby Sanders

Faculty Research Advisors: Dr. Robby Sanders and Dr. Cynthia Rice

The goal of my research is to develop an understanding of the cytotoxicity of polyamidoamine (PAMAM) conjugated dendrimers in cells. This understanding will be carried out by assessing the influence of the cytotoxicity of G4 polyamidoamine-conjugated dendrimers in a cell culture system by using methylthiazolotetrazolium (MTT) assay. It is known that PAMAM dendrimers are slightly less toxic than arginine and ornithine conjugated dendrimers. Knowing the cytotoxicity of dendrimers in cells is important, since polyamidoamine-conjugated dendrimers have the potential as drug carriers to increase the oral absorption of drugs. The cytotoxicity of dendrimers will be tested in vitro via MTT assay. The viability of cells exposed to dendrimers will be expressed as a percentage of the viability of cells grown in the absence of dendrimers. The results from the experiment will show that the percentage of viability of cells grown will decrease as the concentration of dendrimers increases after incubation. This trend also means that the toxicity increases as well.

### IMPROVED SEPARATION TIME FOR BIODIESEL BY MICELLAR SIZE REDUCTION

Jessica Jones

Faculty Research Advisors: Dr. Pedro E. Arce and Dr. Jeff Thompson

Collaborator: Dr. Jeff Thompson

With the price of petroleum fuels rising and the increasing fear of global warming, the search for alternative fuels has rapidly become one of the most prevalent topics in the world today. Biodiesel is one of the most common alternatives; however, the price and availability of reactants and the separation time of the process are the most common obstacles in producing it at an industrial level. Typical biodiesel separation time is approximately twenty four hours. The reaction and separation time can be improved by introducing a wire mesh to the process that will reduce the size of the micelles at which the reaction is taking place. Experiments were performed with three different mesh sizes and samples were taken at given intervals to compare the infrared spectrum for glycerol content. It was found that a smaller micelle will increase the surface area, allowing for a more thorough mixing of the reactants. This will in turn, decrease the separation time between the biodiesel and glycerol layers to less than two hours, drastically increasing the efficiency of the process.

## SUTURE DESIGN TO PROMOTE WOUND HEALING

Stephanie Knowles  
Faculty Research Advisor: Dr. Robby Sanders

Suturing, by a technical definition, is the stitching of tissue with needle and suture material that acts as "thread". In practice, this technique requires as much finesse as a craft such as needlepoint. A comprehensive review of the literature reveals insight regarding types of suturing materials as well as the effect that different suturing techniques can have on scarring and healing of the tissues being joined. Mathematical models have been developed to help predict subsequent scarring in wounded tissues, particularly skin, however no such models have been found that can be used to predict the wound healing process following placement of sutures. Novel models could be developed to: 1) predict which suturing technique best suits a particular wound and 2) predict new methods and materials for suturing to facilitate wound healing and minimize scarring. With reference to needlepoint, the suturing materials create a masterpiece of connected and seamless tissue, just as a picture could be created with the craft. Knowledge of how certain materials affect specific tissues provides insight to how a wound will heal, and this knowledge could be used in modeling to help predict which suturing technique would best suit a specific procedure. Such is the basis for follow-up studies to be conducted.

## CONTACT ANGLE STUDY OF P3HT/PCBM FILMS

Luke Mirtes and Dr. Holly Stretz  
Faculty Research Advisor: Dr. Holly Stretz  
Collaborator: Preejith Ambuken

In the study of polymer based organophotovoltaic solar cells, the dispersion of the fullerene based nanoparticle phenyl-C61-butyric acid methyl ester (PCBM) in the photoactive polymer poly-3hexylthiophene (P3HT) is an important aspect of the cell's overall efficiency. The literature suggests that when these films have their crystals "erased" and then reformed (the process of annealing), the PCBM nanoparticle can aggregate at the surface of the film. In an attempt to clarify the behavior of the surface of these P3HT/PCBM films, we are using contact angle to detect presence of PCBM on the top of the film. The contact angle is measured by dropping a 5 -7 uL drop of water onto the surface of the film and then using a camera and lens to produce a digital image. Images are then imported into the CAD application Draftsight, where the angles are measured manually. The experiment consists of contact angles for known PCBM and P3HT films (~50 nm thick) spin coated on a glass surface, and then comparison of a number of CO<sub>2</sub> (the solvent)

processed films. The hypothesis is that the contact angle of the annealed films will be either close to that of the pure P3HT film or the pure PCBM film, potentially indicating the composition of the film's surface.

## THE IMPACT OF SULFATED ZIRCONIA ON THE CATALYST LAYER OF PEMFCs

William Clark Mitchell  
Faculty Research Advisor: Dr. Cynthia Rice

Proton Exchange Membrane Fuel Cells (PEMFCs) are a possible alternative energy source for the automotive industry, fed with humidified H<sub>2</sub> and air (21% O<sub>2</sub>) with water as the only byproduct. PEMFC's deliver high power density and offer the advantages of low weight and volume. PEMFC's use a solid polymer as an electrolyte and porous carbon electrodes that contain a platinum catalyst. The hydration of the membrane and attached catalyst layers are critical for performance and durability, ancillary saturator are used to pre-hydrate the feed gases, which adversely adds parasitic losses due to increased system weight. My goal is to analyze the impact of Sulfated Zirconia under layers on the cathode platinum catalyst layer level of hydration. Sulfated Zirconia is a super acid and expected to facilitate water retention around the membrane and catalyst layer. The Sulfated Zirconia is added between the cathode and electrolyte. Sulfated Zirconia is highly functionalized inorganic filler that has the properties of water retention as well as proton conductivity. To quantify the impact on hydration and performance several metrics are analyzed; Current Voltage performance on the H<sub>2</sub>/Air fuel cell, Cyclic Voltammetry accessible surface area, and Electrochemical Impedance Spectroscopy of proton resistance in the catalyst layer. The analyzed results have given the conclusion that with greater the weight % of Nafion to Sulfated Zirconia added, the better the fuel cell performs. The cell shows less resistance and greater conductivity.

## EFFECTS OF GOLD NANOPARTICLES IN POLYACRYLAMIDE GEL ELECTROPHORESIS

Jaime Morrison and Dr. Holly Stretz  
Faculty Research Advisor: Dr. Holly Stretz  
Polyacrylamide gel electrophoresis (PAGE) is used in many applications in medical diagnostics. Gold nanoparticles have been shown to help improve the quality of protein separations using PAGE, but these nanoparticles may themselves be moving under the influence of the electrical field. This study will focus on varying electric fields through PAGE and the movement of free nanoparticles through the gel as a result. The gel will be cast in a standard way and then nanoparticles will be electrophoresed at different voltages. Finally the gels will be imaged using a standard digital camera and copy stand and the images analyzed for

distance traveled (velocity) and band spreading. In theory, since the gold nanoparticles have a known zeta potential, they will move under the influence of the voltage. How far they travel and at what voltage they begin to visibly move will be the focus of this study. The gold nanoparticles chosen (50 nm diameters) are visibly red, and therefore easy to detect. The study to date has been centered on calibration of the technique for synthesizing the gels and practical training in gel imaging. The final results of this work are novel and will have significance for both nanoparticle-modified gels for medical diagnostics as well as in the separation/purification of various sizes of nanoparticles when in a mixture.

### OPTIMIZATION OF THE CHEMICAL PLANT PROCESS: AN ASSEMBLAGE APPROACH

Stephanie Poole and Dr. Pedro E. Arce  
Faculty Research Advisor: Dr. Pedro E. Arce

Optimization and Operations research is a tremendous field due to the fact that it incorporates numerical methods in order to make better decisions. In a chemical plant, there are many processes going on at one time and multiple components working together. However, it is largely unknown whether or not a particular reactor or process dominates overall, or if the components work symbiotically to benefit or damage the overall plant operation. Thus, an "Assemblage View" would be useful to learn more about their role in controlling the plant dynamics. Therefore, the motivations of this project are to learn if there are dominating components and then learn how to optimize those aspects. Concepts such as Eigen values, Eigen functions, and the overall Sturm-Liouville Boundary Value problem (SL-BVP) integrated into the frame of "Linear Operator-Method Approaches, LOMA" plays an important role in order to learn where these maximum and minimum points would exist. This presentation will use illustrations from simple cases such as reactors with catalytic pellets in order to develop a basis understanding of more complex systems.

### ELECTROKINETIC SEPARATION OF HEAVY METALS IN POROUS MEDIA: AN EXPERIMENTAL APPROACH

Ms. Kathryn Shpik and Mrs. Rocio Tijaro  
Faculty Research Advisors: Dr. Pedro E. Arce and Dr. Holly Stretz  
Collaborator: Rocio Tijaro

Leaching of some mining byproducts has been linked to human health issues. This project will study the behavior of charged contaminants like copper, lead, and arsenic as they move through porous media similar to soils. The project has specific relevance for heavy metal contamination

of the ground water in areas where the metallic mining industry is prevalent. The objective is to explore the effects of different kinds of external fields (hydrodynamic, electric and a combination of both) on the diffusivity coefficients of the charged heavy metal particles in the saturated porous media. The electrolyte concentration will be varied in order to measure its effects on the diffusivity coefficients. By emulating the experimental design after a traditional Hele-Shaw cell, the first ever experimental results will be generated for radial diffusion of a charged solute. Measurements will be taken to find the effective mass diffusion coefficient in model soils to test the rate of contaminant spreading. The fundamental equation is Fick's Law ( $J_i = -D \frac{\partial C}{\partial x}$ ), the first experiment will focus on the motion of contaminant along  $r$ , radial distance that the species travels over time. Image analysis software will be used to measure the charged particles in terms of concentration (intensity) versus position and time. Electrical fields can be imposed in these types of cells model low Reynolds number; constant flow, constant density, and one-dimensional flow are usually assumed. This project complements the research of Rocio Tijaro, a PhD student in Chemical Engineering.

### RELATING MODELS OF WOUND HEALING TO OTHER REAL WORLD APPLICATIONS

Christian Taylor  
Faculty Research Advisor: Dr. Robby Sanders

Can mass transfer models of wound healing be used to describe other processes such as tire deterioration prevention? The oils in a tire are there to be oxidized instead of the tire being oxidized which would create cracks and weakening the tire. Thus, an assembled tire is designed for self-protection. Tissues are scaffolds of "fibers", cells, and other components that create an environment of homeostasis. In cases of injury, a number of molecules and cells migrate into wounds creating a matrix that fills the wound. This comparative study is being conducted to determine the types of similarities that might exist in these seemingly disparate processes. A review of the literature has revealed papers relating the formation of blood clots in the wounds and the initiation of the wound healing process. While fewer research articles have been found regarding built-in tire protection mechanisms, the search still continues in an effort to find relevant literature describing the way that oils in the tire can be oxidized instead of the tire itself being oxidized. Such approaches can be powerful learning experiences because the analogies that are identified create an expanded knowledge base that is useful in solving problems by relating things to each other. This poster will showcase comparative real-world examples of interest to mass transfer.

## CIVIL AND ENVIRONMENTAL ENGINEERING GRADUATE STUDENTS

### IMPACT OF CONSIDERING FLOW VELOCITY AND INUNDATION DURATION IN FLOOD MANAGEMENT DECISIONS

Ebrahim Ahmadisharaf  
Faculty Research Advisor: Dr. Alfred Kalyanapu

A comprehensive insight about hydraulic characteristics of floods is needed to select the most suitable strategy for flood risk management. This evaluation is generally performed based on the floodwater depth. In other words, decision criteria such as structural damages are also appraised as a function of inundation depth. Other flood parameters such as flow velocity and duration of flooding are rarely taken into account. This may result in selection of a flood management with the lowest flood depth magnitude regardless of consideration of flood velocity and duration. Therefore, this raises uncertainties in assessment of flood management options. This study investigates the impact of consideration of these parameters on flood management decisions. An integrated approach is represented for assessment of flood management options. The approach employs a two-dimensional flood model, Flood2D-GPU, for flood modeling and a spatial multi-objective decision analysis (SMODA) tool, spatial compromise programming (SCP) for evaluating flood control alternatives. Applying Flood2D-GPU provides comprehensive information about flood depth, velocity and duration. Here, four attributes, including inundation depth, velocity and duration as well as structural damages are considered for assessment of feasible flood control alternatives. Simulated flood parameters are used to estimate flood damages using depth-damage relationships and land use layers. The presented SMODA is demonstrated on the Swannanoa River Watershed, located in the upper Tennessee River region in Buncombe County, NC.

### DEM CORRECTION ALGORITHM TO DERIVE SYNTHETIC CROSS SECTIONS FOR FLOOD INUNDATION MODELING

Md. N. M. Bhuyian and Dr. Alfred J. Kalyanapu Faculty  
Research Advisor: Dr. Alfred Kalyanapu

Digital Elevation Model (DEM) is an important dataset for flood modeling and simulation. Advanced remote sensing technology has made elevation data available for remote areas. So far the DEMs generally available like the National Elevation Dataset (NED) do not provide accurate elevation information of the surface below the water bodies. Several researchers have proposed methods to solve this problem

by applying simple prismatic cross sections or removing unusual spikes or noises along the streamlines. These methods did not take the site specific geomorphologic conditions into consideration such as planform, thalweg, meander etc., rather they used synthetic and prismatic sections and would take open channel conditions into consideration. In this research, we developed a DEM adjustment algorithm that incorporates the planform and morphologic characteristics of channel along with open channel flow conditions. For each cross section the locations with the steepest slope at the left and right are selected as left high bank and right high bank. It was assumed that for a single channel river the location of deepest point (thalweg) is close to the outer bank in a meandering channel. The intersection of left and right slopes is considered the location of thalweg. Using Manning's equation the uniform flow depth was calculated. Reference discharge corresponds to the flow at water surface elevation equal to the elevation available in the DEM at the gage location. Uniform depth for each cross section were calculated separately. Study area is Cumberland River. Simulation of high and low flow events have shown good agreement with observed scenario.

### DEVELOPMENT OF LEACHATE TEST FOR DELAYED ETTRINGITE FORMATION POTENTIAL IN CEMENTITIOUS MATERIALS

Jojo France-Mensah  
Faculty Research Advisor: Dr. Benjamin Mohr

Concrete is the most widely produced man-made material in the world. Annual global production of concrete is estimated to be about 5 billion cubic yards. The need for an early strength gain of concrete and ultimately faster construction has led to the increased application of steam curing to concrete. This can lead to a durability problem in concrete called delayed ettringite formation (DEF). Previous research has shown DEF to be responsible for expansion and cracking in later ages of concrete. The existing method of measuring expansion caused by DEF takes at least a year to obtain any significant results. It has been proven that the leaching of alkali ions (e.g., sodium and potassium) from the cement matrix accelerates the rate of expansion through DEF. It has also been noted that after heat curing, the adsorbed ions (e.g., calcium, sulfates and aluminates) are released and become soluble in the pore solution. The relevant ions to DEF formation are going to be leached out of concrete and the results correlated to expansion results of similar samples studied earlier. The research aims to use this knowledge to develop an accelerated leachate test method to identify the potential use of DEF in cement-based materials in order to decrease the time compared to the existing method.

## SATELLITE RAINFALL UNCERTAINTY ESTIMATION FROM READILY AVAILABLE GEOPHYSICAL FEATURES AND RAINFALL RATE

Abebe Gebregiorgis  
Faculty Research Advisor: Dr. Faisal Hossain

Nonlinear regression model is used to fit the response variable of three satellite rainfall error variance (3B42RT, CMORPH, PERSIANN-CCS) with explanatory variable (satellite rainfall rate) by grouping them as function of three key geophysical features: topography, climate, and season. The results of the study suggest that the error variance of a rainfall product is strongly correlated with rainfall rate and can be expressed as a power-law function. The geophysical feature based error classification analysis helps in achieving superior functional accuracy for prognostic error variance quantification in the absence of ground truth data. The multiple correlation coefficients between the estimated and observed error variance over an independent validation region (Upper Mississippi River basin) and time period (2007 – 2010) are found to be 0.75, 0.86, and 0.87 for 3B42RT, CMORPH, and PERSIANN-CCS products, respectively. In another validation region (Arkansas-Red River basin), the correlation coefficients are 0.59, 0.89, and 0.92 for the same products, respectively. Results of the assessment of error variance models reveal that the type of error component present in a satellite rainfall product directly impacts on the accuracy of estimated error variance. The model estimates the error variance more accurately when the precipitation error components are mostly hit bias or false precipitation, while for a product with extensive missed precipitation, the accuracy of estimated error variance is significantly compromised. The study clearly demonstrates the feasibility of quantifying the error variance of satellite rainfall products in a spatially and temporally varying manner using readily available geophysical features and rainfall rate.

## USE OF SUPERABSORBENT POLYMERS AS PHYSICAL AIR-ENTRAINER WITH USE OF MARGINAL FLYASH

Jared Thompson  
Faculty Research Advisor: Dr. Benjamin Mohr

There are durability issues for concrete that cause failure. Cyclic freezing and thawing is one of the durability issues and it can be mitigated by the use of air-entraining admixtures. These chemical admixtures allow the formation of air bubbles in the concrete to help reduce the degradation of the cyclic freezing and thawing. Fly ash is a byproduct of pulverized coal combustion and it is used in concrete to make it more economical. There are different types of fly ash and they are Class C and F and these are commonly used. The Environmental Protection Agency limits

the amount of nitrogen oxide emissions produced from coal combustion and this affects fly ash that is being produced. Because of these limitations there is another type that is not used in concrete and it is disposed of in landfills and it is called marginal fly ash. The marginal fly ash has high carbon content and it acts like an active carbon. It will absorb the chemical air entrainers that are used to prevent freezing and thawing degradation. Superabsorbent polymers (SAP) are polymers that can absorb water. The SAP can be used in concrete as a physical air entrainer. As the concrete hardens and water is removed from the SAP, the polymers will decrease in size leaving behind an air void. Therefore, the purpose of this research is to compare chemical and physical air entrainers with the use of marginal fly ash.

## COMPUTER SCIENCE GRADUATE STUDENTS

### DETECTING ANOMALY IN SMART METER DATA

Vitaly Ford and Dr. Ambareen Siraj  
Faculty Research Advisor: Dr. Ambareen Siraj

The Smart Grid will gradually replace legacy Power Systems with more advanced, reliable, and manageable technologies. However these new technologies like the smart meters require elaborate security analysis for preventing malicious attacks and preserving confidentiality and integrity of consumer data. Our research analyzes Smart Meter data for learning normal consumer usage of electricity and then uses the acquired knowledge to detect any anomalies in user consumption -thus addresses the problem of Smart Meter data forgery. The Smart Meter data under investigation consists of actual Electricity Customer Behavior information, shared by the Irish Social Science Data Archive center. We are employing machine learning techniques such as Neural Network and Support Vector Machines to learn usage profiles from smart meter data.

### MOBILE AGENT BASED ARTIFICIAL IMMUNE SYSTEM FOR INTRUSION PREVENTION IN THE CLOUD

Joshua Tower  
Faculty Research Advisor: Dr. Ambareen Siraj

Despite numerous benefits of cloud computing, companies are less willing to move to the cloud because of lack of security controls offered for cloud services. With little to no safeguards to protect confidentiality, integrity, and availability of their information, companies often are not comfortable in placing their sensitive information/important resources in the cloud. In order for the cloud to be widely adopted, security mechanisms must be in place to protect

virtual machines from attack. To address information assurance in cloud, our research proposes a framework for an Active Intrusion Detection System that can protect virtual machines supporting cloud infrastructure from malicious traffic. This system simulates the artificial immune system to differentiate self (benign) and foreign (potentially malicious) bodies in the form of system calls. This system works actively by blocking known malicious system calls from executing. It is also adaptive in that it can accommodate uncertainty through the concept of gray listing. Finally, because the cloud environment is composed of many virtual machines on various physical machines, mobile agents are periodically dispatched to share knowledge about attacks. We believe this system will make the cloud environment more resilient to attacks benefiting both cloud providers and their clients.

## COMPUTER SCIENCE UNDERGRADUATE STUDENTS

### A JAVA TOOLBOX FOR PROGRAMMING MICRO-CONTROLLERS

Adam Shaw  
Faculty Research Advisor: Dr. Shiekh Ghafoor

A micro-controller is a micro-computer used to control physical devices such as robots and machinery. They are similar to desktops, laptops, and supercomputers in that they have memory, a CPU, input devices, and output devices. However, micro-controllers do not have keyboards, hard disks, or large display screens. Instead, they have buttons, a small LCD screen with limited characters, and analog to digital channels (such as reading the light level) for input and output. Micro-controllers are traditionally programmed either in assembly or the C programming language. The traditional entry-level engineering programming courses use Matlab, Java, C, or Fortran. Introductory engineering students expect to learn how manipulate their world as part of their major, but manipulating physical objects with assembly is of senior level difficulty. This project presents a toolbox that meets their expectation of allowing them to control new hardware, but in an environment they are familiar with. Specifically, this toolbox enables students to program a Dragon-12 micro-controller using the Java programming language. It has been in use at Roane State Community College since fall 2012 to teach programming.

## ELECTRICAL AND COMPUTER ENGINEERING GRADUATE STUDENTS

### CONTROL AND OPTIMIZATION MECHANISMS OF A GENERIC VIRTUAL POWER PLANT

Brook Workneh Abegaz  
Faculty Research Advisor: Dr. Satish M. Mahajan

The obvious advantage of the integration of distributed energy resources (DERs) from various distributed generation units (DG) into the utility power grid is that such energy resources can support a significant share of the total power load and that they can help reduce transmission power losses. However, since DERs are often small in capacity and numerous to be manageable on an individual basis, the virtual power plant (VPP) concept is required to counteract this problem by aggregating individual DERs into transmission-connected generation-sources. A generic virtual power plant (GVPP) has many influential characteristics such as aggregating the capacity of numerous distributed energy resources (DERs) dispersed among the power network at medium voltage and low voltage levels and creating a single operating profile from a composite of parameters characterizing each distributed energy resource (DER). Furthermore, the aggregation of such DERs into a virtual power plant brings forth a change in the conceptual framework of electric power systems in that the ICT infrastructure of virtual power plants could help in the smooth transition of the current passive distribution network into an active network. Topics addressed in this research include the design of aggregation and control mechanisms of Distributed Energy Resources (DER) (DG + DS) into a Virtual Power Plant, followed by identification of the voltage and power characteristics (both active and reactive) of the virtual power plant when connected to the main grid. The research is implemented using Matlab-Simulink simulation of a virtual power plant using induction machines, synchronous machines, and different excitation models. Moreover, the research aims at increasing the stability and reliability of the generic virtual power plant and thus the overall power grid operations through specific kind of power flow controllers.

### SYNTHESIZING AND INTEGRATING TSE WITH HARD CORE TCP/IP FOR SMART GRID

Rami Amiri and Dr. Omar Elkeelany  
Faculty Research Advisor: Dr. Omar Elkeelany

Embedded systems are categorized into general-purpose processors (GPP), application-specific instruction set processor (ASIP) or custom single-purpose processor (CSPP). TCP/IP processing is being off-loaded onto either general-purpose processor (GPP), or application-specific instruction-set processor (ASIP). But TCP/IP has not been designed/ off-loaded as a custom single-purpose processor (CSPP) yet. Both implementations; GPP and ASIP execute TPC/IP as a software core which are mainly instruction based. In this research we aim to design a new custom single-purpose processor to off-load TCP/IP using CSPP technology.

## CONCURRENT RECONFIGURABLE ARCHITECTURE FOR MAPPING AND ENCRYPTING A MESSAGE IN ECC

Rami Amiri and Dr. Omar Elkeelany  
Faculty Research Advisor: Dr. Omar Elkeelany

Elliptic Curve Cryptography (ECC) over a GaloisField GF ( $2^m$ ) offers a high security level relative to other protocols (i.e., RSA) but with smaller keys' sizes. In this paper, we consider the finite field multiplication and addition used in elliptic curve cryptography to design sequential, and then, concurrent reconfigurable crypto system to encrypt and decrypt a message. FPGA implementation via VHDL language has been completed to analyze the time and area required in both scenarios. Our approach is novel in that we consider mapping a message on the elliptic curve concurrently.

## A THREE AGENT SMART GRID SYSTEM

Adeniyi Babalola and Viraj Anagal  
Faculty Research Advisor: Dr. Rabie Belkacemi

The possibilities of the smart grid are numerous and the future of energy generation, transmission, distribution, consumption and sales is largely dependent on the progress made in smart grid technology. Some of the areas where such progress is expected are in the control and self-healing abilities of agents connected to the grid due to the dynamics of the power grid. In this research work, two three-phase generator systems, one of ratings 208V, 1.7A and 246W while the other is 220V, 1.7A and 246W, are connected through a three bus system to a variable load system through a 10 $\Omega$ , 1mH and 3-5 microfarad transmission line. The set-up is synchronized and controlled using shared variables. This research then looks into the self-healing abilities of this three agent smart grid system. Power at some parts of the system is varied and the response of the system to these variations is as to neutralize the effect of the variations.

## AUTOMATED EXPERIMENTAL DATA COLLECTION SYSTEM FOR RADIO TOMOGRAPHIC IMAGING

Jason Bonior and Dr. Zhen Hu  
Faculty Research Advisors: Dr. Robert C. Qiu and Dr. Nan Guo

Radio tomographic imaging is the process of constructing images based on changes in signal amplitude and phase between nodes within a wireless system. In the pursuit of the realization of a radio tomography system we have constructed an automated system for data collection. Through our research, this system allows for the collection

of high-quality data which can be used to test imaging algorithms. Our system includes an RF-anechoic chamber, turntable, vector-network analyzer, software-defined radios, and a LabVIEW control program running on a server. Custom parts (antenna mounts, etc.) were designed using 3D-CAD software and constructed using our state-of-the-art 3D printer. We will present our system and discuss how the collected data will be used to support our group's research.

## EXPERIMENTAL DEMONSTRATION OF COGNITIVE RADAR FOR TARGET LOCALIZATION UNDER STRONG INTERFERENCE

Xia Li and Zhen Hu  
Faculty Research Advisor: Dr. Robert C. Qiu

One of the major objectives of cognitive radar is to form a dynamic closed feedback loop to adapt the spectrum of transmit waveforms to avoid certain interference. For this paper, we built an automatic closed-looped cognitive radar to support experimental study of radar systems in real-world situations. Convex optimization was applied to jointly design sounding waveforms and matched filters with spectral power suppressed in arbitrary bands and with low correlation sidelobes. Target localization is demonstrated under strong interferences. Experimental results are provided to evaluate the performance of the cognitive radar system.

## TRANSIENT STABILITY ANALYSIS OF A MULTI MACHINE POWER SYSTEM

Waheed Oyekanmi  
Faculty Research Advisor: Dr. Ghadir Radman

Transient stability analysis has recently become a major issue in the operation of power systems due to the increasing stress on power system networks. Stability is an important concept which determines the stable operation of power systems. This problem requires evaluation of a power system's ability to withstand disturbances while maintaining quality of service. Many different techniques have been proposed and applied to the problems of transient stability in power systems, especially for multi-machine systems. These methods include the time domain solutions, the extended equal area criteria, and the direct stability methods such the transient energy function. However, the most methods must transform from multi-machine system to an equivalent machine and infinite bus system. In this research work, a method as an accurate algorithm to analyze transient stability for power system for an individual machine is put forward. It is a tool to identify stable and unstable conditions of a power system after fault clearing

with solving differential equations numerically. This method is performed on six-bus power system.

## ARQ BASED SOFT ERROR TOLERANT DATA PATHS FOR SRAM-BASED FPGAS

Phani Balaji Swamy Tangellapalli and Dr. Syed Rafay Hasan  
Faculty Research Advisor: Dr. Syed Rafay Hasan

The SRAM-based FPGA, due to their high performance, has become a popular choice in today's electronic systems and are used in large number of applications. But in radiation harsh environment these FPGAs require some additional mechanism to cope up with soft errors. Modern FPGAs are built in 28nm technologies, where even combinational circuits are substantially vulnerable to soft errors. Such designs require soft error mitigation circuits in their data paths. Conventional soft error mitigation techniques such as triple modular redundancy are robust but their area overhead is three times as compared to normal design. In this paper a variant of automatic repeat request (ARQ) protocol is proposed, along with delayed redundancy to reduce area overhead. Synthesis results show an improvement of 9.1 and 10% in latency for Cyclone II and Stratix II FPGAs, respectively, with a 1.94 times improvement in resource utilization. Our synthesis results show that our implementation is not only better in terms of area overhead but if a soft error occurs once in 10 clock cycles the overall system throughput is better for the proposed architecture compared to TMR. To our knowledge this is the first work to implement ARQ based protocol utilizing delayed redundancy to mitigate soft errors in SRAM-based FPGAs.

## LARGE SCALE COGNITIVE RADIO NETWORK TESTBED

Changchun Zhang and Feng Lin  
Faculty Research Advisor: Dr. Robert C. Qiu

The cognitive radio technology is emerging technology that enables smart and intelligent next generation users of wireless communication networks to tap into the significantly improved utilization efficiency of the radio spectrum. On the other hand, the radio resource management via cross layered optimization provides the network with more flexible, efficient communications. The critical steps to an intelligent network are the statistical data collection and processing within cross layers. After years of pioneer theoretical research in the key areas of cognitive radio, the Cognitive Radio Institute of TTU is now building a large scale cognitive radio network testbed, which is developed over state-of-art Software Defined Radio platform-USRP. This large scale network testbed will be composed of more than 80 radio nodes, to pursue the Big Data which reveals more information of the network behaviors and radio

environment. Different network topologies, like centralized manner or Ad-Hoc manner, are explored. Parallel computing is also integrated into the signal/data processing blocks to accelerate the stream based real-time processing. This large scale network testbed will become an impressive research platform to verify the theoretical algorithms, discover the real phenomenon, by the real Big Data in the cognitive radio network.

## ELECTRICAL AND COMPUTER ENGINEERING UNDERGRADUATE STUDENTS

### COOPERATIVE ANALOG WIRELESS SENSOR NETWORKS: A LOW-COST APPROACH FOR PARALLEL SCENARIOS

Gus Gillen  
Faculty Research Advisor: Dr. Adam Anderson

There is a great need for inexpensive, wireless sensor networks. Being able to control and monitor everything around us drives and facilitates our research. In a world constantly growing more dependent on technology, we are always searching for more cost effective ways of examining the world around us. We are developing an analog wireless sensor capable of mass production with the ability of parallel operation. This device should be cheap enough to manufacture en masse and be able to transmit the signal produced by the sensor in the analog domain. The signal transmitted is a steady analog waveform, modulated by information with approximately static values like

temperature, acoustics, or radiation; things that can change but will stay at roughly constant values over an extended period of time. The data pulse will contain a training voltage, an individual ID voltage, and the actual sensor information. The measured values will change slowly with respect to time and therefore the transmitted messages should use low bandwidth. We will be looking at factors such as signal to noise ratio (SNR), spectrum efficiency, range, cost, and size compared to a similar digital WSN in hope of constructing a more accurate analog transmitter than an equivalent digital signal while at a lower cost.

### INSTANTANEOUS FREQUENCY DIVISION MULTIPLEXING: AN APPROACH FOR WIRELESS HIGH-DEFINITION VIDEO

Dennis Ogbe  
Faculty Research Advisor: Dr. Adam Anderson

In LESS surgery, doctors perform an entire surgical procedure through one small incision, usually the navel.

This procedure is much less traumatic on the body and leaves the patient without a scar. To perform this surgery wired endoscopes and surgical tools self-interfere while inserted into the single incision. A wireless approach to high definition scopes will prove invaluable to surgeons. Since the surgeon has only one small incision to work with, there is a need to use the minimal opening more efficiently along with a higher resolution video. A few ways to make this procedure more efficient are to make the cameras wireless and make the video high-definition. This project will present a new analog modulation and multiplexing technique for wirelessly transmitting high-definition video using hardware which is smaller in size and less expensive than a comparable digital system. High-definition video can be transmitted wirelessly using a new analog modulation scheme which will be referred to as instantaneous frequency division multiplexing. Each video component is frequency modulated and then transmitted. The receiver will utilize a phase-locked loop to track the orthogonal instantaneous frequencies. Unlike frequency division multiplexing which requires each signal to occupy separate frequency bands, the use of orthogonal instantaneous frequencies allows the video components to occupy the same bandwidth. The IFDM technique will be demonstrated through simulation and a prototype hardware implementation. It is expected that the performance of this system will be comparable to digital modulation schemes.

## **MANUFACTURING AND ENGINEERING TECHNOLOGY UNDERGRADUATE STUDENTS**

### **PRODUCTION OF BIODIESEL FROM WVO USING SMALL SCALE CONTINUOUS ULTRASONIC PROCESSOR**

Justin Wood, Jared Slayton, and Seth Parrott  
Faculty Research Advisor: Dr. Ahmed Elsayy

There is a need in the USA to decrease dependency on fossil fuels. One alternative fuel that has gained much popularity in the past few years is biodiesel. Biodiesel can be produced using vegetable oil, waste vegetable oil (WVO), animal fat and yellow grease as raw materials. However, the process of converting a batch of WVO into usable biodiesel is time consuming, requires a human operator to run the system, and necessitates the performance of a chemical titration for each batch of biodiesel produced. In the first phase of this project, the processor was designed and built by the senior design students utilizing a programmable logic controller (PLC) in conjunction with pumps, valves, temperature sensors, etc. to completely handle the production of

biodiesel with minimum operator interaction. This was the first step toward continuous flow processor and the elimination of the titration process. In the second phase of this project, the students integrated a small Hielscher Ultrasound continuous processing unit to the automated system. This paper presents the newly developed system and demonstrates the design aspects of the automated biodiesel production processor using a PLC and ultrasonication (continuous processing) as well as how the chemical titration procedure for each batch is eliminated.

## **MECHANICAL ENGINEERING GRADUATE STUDENTS**

### **AN OPTIMAL POWERTRAIN CONTROL STRATEGY FOR A MILD HYBRID ELECTRIC VEHICLE**

Jeff McGehee  
Faculty Research Advisor: Dr. Sally Pardue  
Collaborator: Dr. Hwan Sik Yoon (University of Alabama)

As a viable alternative to the conventional hybrid electric vehicles, so called "mild" hybrid drive trains are currently being implemented in production vehicles. These mild hybrid electric vehicles use an Integrated Starter Generator (ISG) to simply assist the internal combustion (IC) engine rather than drive the vehicle independently of the IC engine. Some of the production mild hybrid vehicles have been shown to achieve over a 10% increase in fuel efficiency with minimal additional costs. In this paper, we present a lookup table-based control scheme for the optimal control of the ISG and the IC engine on a mild hybrid vehicle. The developed control logic is implemented in Matlab/Simulink along with a mild hybrid vehicle model, which is based on an EPA light-duty vehicle model. The simulation results show that the optimally controlled mild hybrid vehicle has better fuel efficiency with comparable drivability when compared to a simple intuitive rule-based control strategy.

### **CONJUGATION DESIGN, PROTOTYPING, AND TESTING OF HARMONIC DRIVES**

Zhiyuan Yu and Jacob Sands  
Faculty Research Advisor: Dr. Kwun-Lon Ting

Harmonic drive is a special mechanical gear system with a very high speed reduction ratio, high torque-to-weight ratio within an extremely compact volume, so HDs are key elements for motion control application with strict space requirement, for instance, lunar vehicles, robot joints, aerials, telescopes, numerical control machine tools. The objective of the proposed research is to offer a general and coherent design methodology for harmonic drives to prolong their

life and enhance the performance under a nominal loading condition. The design methodology lies on two fundamental kinematic principles ignored in the conventional harmonic drives. First of all, the deformation of the HD's flexspline, which essentially controls the flexspline tooth motion, must follow the principle of motion generation in transmission through direct contact. Secondly, the conjugation principle must hold and tooth profiles should be optimized to fit the specific loading condition. A virtual prototype will be developed and improved with ANSYS® explicit dynamics. The specific goal is to check the result of the life time, efficiency, and noise and vibration of the new design. The value of virtual prototype testing at this stage is tremendous in evaluating these potential improvements because of the high cost and time involved in building the huge number of new designs' physical models. Also it can simulate the interactive influence of the flexspline's deformation and the teeth's conjugation under the loading condition. Finally, a physical prototype will be manufactured and tested through an international collaboration with ITRI, and tested for validation.

## MECHANICAL ENGINEERING UNDERGRADUATE STUDENTS

### DEVELOPING METRICS FOR COMPARISON OF MOBILE ROBOTS PERFORMING WELDING TASKS

Kevin Lutz  
Faculty Research Advisor: Dr. Stephen Canfield

Developments in mobile robotic systems are increasing the potential for autonomous robotic systems to make contributions to manufacturing processes that traditionally do not utilize automation. Some tasks in these manufacturing processes require validation before they can be implemented, which is a major obstacle to the use of mobile robotic systems. One example of such a task is welding. Welding processes are designed to satisfy industry standards, such as those developed by the American Welding Society. In many circumstances both the human operator and equipment must be certified. The standards developed by the American Welding Society pre-date the use of mobile robotic welding systems, so robotic systems were not considered in the development of these standards. The goal of our research is to develop a metric that gives a quantitative measure of a robot's ability to weld. This metric is proposed to be used in conjunction with existing American Welding Society's quality standards to validate new robot welding systems. This method focuses on analyzing tasks that can be broken into a short sequence of well-defined motions called gaits that are performed repeatedly or in a periodic manner, such as the motion desired in a welding pattern. In order to develop a quantitative comparison, we propose using a

geometric comparison of the capabilities of the robot to the requirements of the specific welding pattern. This metric will contribute to the design and development of mobile robotic welding systems to become an acceptable and certifiable contributor to the manufacturing processes.

### IMPEDANCE SPECTROSCOPY OF OXIDES FORMED DURING OXIDATION OF COBALT PLATED CROFER 22APU

Albert Painter and Samgopiraj Velraj  
Faculty Research Advisor: Dr. Jaihong Zhu

Solid oxide fuel cells (SOFCs) are a promising alternate fuel energy source for greener power generation. Recent developments have lowered the operating temperature to 600–800C, paving the way for the use of stainless steel as interconnect and reducing the cost significantly. Although Crofer 22 APU has emerged as the most successful interconnect material, protective coatings are needed for better conductivity, reduced scale growth and Cr volatility. The objective of this study is to investigate the oxidation and electrical behavior of cobalt-coated Crofer 22 APU oxidized at 800C for varying time (2 h, 50 h, 100 h and 500 h) in air. Impedance spectra of the oxide film revealed the presence of two or three semicircles depending on the oxidation time, which corresponds to the presence of individual oxide scales. The oxide film was also examined by using scanning electron microscopy (SEM) and X-ray diffraction (XRD). SEM and XRD analysis of the 500h sample clearly showed the presence of three oxide layers (Cr<sub>2</sub>O<sub>3</sub>, CoCr<sub>2</sub>O<sub>4</sub> and Co<sub>3</sub>O<sub>4</sub>). The SEM images of the lesser oxidation time samples did not clearly show the CoCr<sub>2</sub>O<sub>4</sub> layer but the impedance plots implied the presence of a third layer. The oxide scales were assigned to their respective semicircles and the electrical properties of Cr<sub>2</sub>O<sub>3</sub>, CoCr<sub>2</sub>O<sub>4</sub> and Co<sub>3</sub>O<sub>4</sub> oxide scales have been determined by impedance measurements.