# 4th Annual
# STUDENT
# RESEARCH DAY

Research holds the golden key to the discovery of new knowledge in all disciplines

**TTU**
## Tennessee Tech
## UNIVERSITY

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# RESEARCH DAY - PURPOSE

Student Research Day at Tennessee Technological University is an event DESIGNED TO SHOWCASE in a poster format the research and other scholarly activities of undergraduate and graduate students.

# SCHEDULE OF EVENTS

**Student Research Day**
Roaden University Center
Multipurpose Room

**Tuesday, March 31, 2009**

**7:00 a.m. – 8:00 a.m.**      Poster Set-up

**8:00 a.m. – 9:30 a.m.**      Judging
Students at posters (if possible)

**10:00 a.m. – 11:15 a.m.**   Open Poster Review and Discussion
Students at posters (if possible)

**11:15 a.m. – noon**          Awards Ceremony

**Noon- 2:00 p.m.**             Open Poster Review and Discussion
Students at posters (if possible)

**2:00 p.m. – 3:00 p.m.**      Poster pick-up

***Refreshments will be served throughout the day.***

March 31, 2009

Dear Student Investigators:

Congratulations on the outstanding display of investigative research! On behalf of the students, faculty and staff at Tennessee Technological University, I commend you for your research accomplished under the guidance of faculty research advisors. Your participation in Student Research Day brings honor and recognition to yourself, the University, the greater community and to the State. We thank you for sharing your research efforts.

Research is central in University training. Your research displayed today showcases Tennessee Technological University's being named, for five consecutive years, one of the Best Southeastern Colleges by the Princeton Review. U.S. News and World Report ranks Tennessee Tech University in the Top Ten Public Universities in the South – Master's category rankings.

Thank you for participating in Student Research Day!

Sincerely,

Robert R. Bell
President

Dear Tennessee Tech students:

TTU is strongly committed to active forms of learning, and student research, at both the graduate and undergraduate levels, has become one of the key forms. Research 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'm delighted to welcome everyone to Student Research Day 2009, a time for celebrating our commitment to active learning and for showcasing the work of some of our best students.

Sincerely,

Jack Armistead
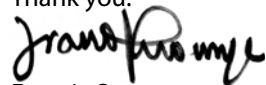Provost and Vice President for Academic Affairs

WELCOME TO TENNESSEE TECH RESEARCH DAY

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 Tech.

Students' participation in research is consistent with our commitment to the life-long 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 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 by the opportunity provided by the Student Research Day for students to showcase their creative endeavors. We hope that the projects would 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

# ACKNOWLEDGEMENTS

# AGRICULTURE
## UNDERGRADUATE STUDENTS

### WATER HOLDING CAPACITY AS INFLUENCED BY ADDITIONS OF COMPOST

Nicholas Mooneyham
Agriculture
Faculty Research Advisor: Dr. Janice Branson

Water holding capacity in soil is an indication of how a particular soil will act under a given set of circumstances. The objective of this study was to determine if there were noticeable differences in water holding capacity of test plots treated with varying amounts of organic compost. Sampling included two replications of each treatment (0 lbs of compost, 22 lbs of compost, 66 lbs of compost, and 110 lbs of compost). Samples were analyzed for organic carbon content, bulk density, and gravimetric moisture. Bulk density in all composted plots was reduced by organic matter additions. While field capacity and saturation measurements reflected a definite influence from organic matter content in the south end of the field, soil inconsistency at the north end resulted in a high amount of variability in those plots.

### THE EFFECT OF COMPOST APPLICATIONS ON EARTHWORM POPULATIONS

Aurora Scott
Agriculture
Faculty Research Advisor: Dr. Janice Branson

Aristotle once referred to earthworms as "the intestines of the Earth". Earthworms are a critical component decomposition of organic materials in the soil ecosystem. The objective of this study was to determine if varying rates of compost resulted in a corresponding increase in earthworm population. At the TTU Water's Farm, eight 18"x18"x 6" soil samples (two replications) were taken from tomato plots. Each plot had received one of the following treatments:  0 lbs, 22 lbs, 66 lbs, or 110 lbs of compost. All soil in the samples was sifted with a 2 mm sieve. Earthworms were extracted during the sieving process. Plots containing 0 compost contained 43 earthworms, populations in plots with 22 pounds of compost increased by 121% (95 earthworms), populations in plots with 66 pounds of compost increased by 86% (80 earthworms), and populations in plots with 110 pounds of compost increased by 63% (70 earthworms). While there was a definite increase in populations in plots receiving additional food material, the higher rates of compost additions did not result is a corresponding increase in earthworm population. Therefore, additional compost would have limited results concerning earthworm population.

### ROOT YIELDS IN COMPOSTED TOMATO BEDS

Lance Yates
Agriculture
Faculty Research Advisor: Dr. Janice Branson

Organic compost improves soil quality resulting in greater concentrations of root material. High levels of organic matter in soil improve permeability, water holding capacity, and bulk density. The objective of this study was to determine the concentration of roots in seven plots with different amounts of compost applied to each plot. An 18" x 18" x 6" sample was removed from each plot using a sod cutting shovel. Soil was separated from roots with a 2 mm sieve and the roots then washed. Roots were sorted by size (very fine, fine, medium, coarse, and very coarse) and weighed. Results showed sample 89-T-3 receiving 66 lbs. of compost per plot had the greatest concentration of root material present. Samples with concentrations of 110 lbs. showed a significantly lower amount of root material in comparison. Plots receiving 0 or 22 lbs. of compost varied greatly in root concentration.

# HUMAN ECOLOGY
## UNDERGRADUATE STUDENTS

### CURRENT RESEARCH ON THYROID DISEASE

Crystal Johnson
Human Ecology
Faculty Research Advisor: Dr. Melinda Anderson

The purpose of this current research project is to provide general information concerning the thyroid glands as well as the hormones/functions, problems/disorders, deficiencies and symptoms/treatments of the glands. The endocrine system consists of eight main endocrine glands that secrete hormones. Specifically, the thyroid gland, its hormones/functions, problems/disorders, deficiencies and symptoms/treatments will be covered. Simply, the thyroid hormones, T3 and T4, regulate metabolism. Some problems and disorders associated with the thyroid are hypothyroidism, Hashimoto's thyroiditis, hyperthyroidism and Grave's disease. Hypothyroidism is a result of an under-active thyroid gland not producing enough thyroid hormone. Hyperthyroidism occurs from an overactive thyroid gland that produces too much of the thyroid hormone. Some symptoms associated with hypothyroidism are fatigue, weight gain and feeling cold. A few symptoms of hyperthyroidism are weight loss, diarrhea and even infertility. Treatments vary among each disorder. One deficiency linked to the thyroid gland is goiter, which is merely an enlarged thyroid gland that physically proves the thyroid is growing abnormally. Proper functioning of the thyroid gland is crucial to ones health and plays a vital role in the body.

## DIABETES AND INTENSIVE THERAPY

Felicia Shoulta
Human Ecology
Faculty Research Advisor: Dr. Melinda Anderson

According to the American Diabetes Association 17.5 million Americans have diabetes. Along with diabetes also come serious complications. Diabetes and diabetes-related complications account for more than 174 billion dollars in healthcare costs each year! Two types of diabetes exist. Type one is also known as insulin-dependent diabetes mellitus which means that the pancreas no longer produces insulin. It usually occurs in children and adolescents. It is unknown what causes type one, but it may be linked to genetics. Type two diabetes is the most common type and usually occurs in older adults (recently many children are diagnosed due to obesity). Heart disease, kidney disease, eye problems, and nerve damage are just a few of the complications that can occur due to uncontrolled diabetes. The goals of treating diabetes is getting blood glucose as close to normal as possible and to prevent future complications. The Diabetes Control and Complications Trial (1983-1993) studied how well intensive therapy reduced diabetes-related complications. Intensive therapy consisted of 3-4 injections of insulin a day, individual consultation, frequent blood glucose tests, and a goal of close to normal blood glucose levels. Intensive therapy appeared, and continues, to be the best at controlling diabetes and preventing complications.

## THE EFFECT OF WHOLE WHEAT FLOUR ON BANANA MUFFIN QUALITY

Mary Walker Watson and David Knieling
Human Ecology
Faculty Research Advisor: Dr. Cathy Cunningham

The purpose of this experiment was to measure the effect of whole wheat flour on taste and nutrient content of banana muffins. Increasing consumption of whole grains has a positive effect on health. The banana muffins were made in three treatments varying the ratios of all-purpose and whole wheat flour (66%:33%, 50%:50%, 33%:66%). Banana muffins were evaluated by ten panelists for internal air cell size, internal color, flavor, moistness, and overall acceptability. Internal color and internal air cell size scores were more significantly different than moistness and taste scores. Two trained food scientists found no difference when evaluating the appearance of the internal crumb. Each muffin treatment was measured objectively for height, weight, nutrients and cost. There was no significant difference in height, weight or cost of the banana muffins.

# CHEMISTRY
## GRADUATE STUDENTS

## ASSEMBLING A FLOW-CELL FLUORESCENCE SENSOR FOR COPPER, ZINC AND ALUMINIUM USING POLYMER MEMBRANE

Henry Abougor, Sarah Brinkley, John Patridge, Matt Mancuso and Roshan Fernando
Chemistry
Faculty Research Advisor: Dr. Andrew F. Callender

The rising problem of pollution in our environment has prompted the need for sensitive device, able to detect trace amount of metal ions in the environment. We have developed a compact, portable fluorescence sensor for rapid screening of metal ions in polluted waters. The sensor consists of am ion-selective fluorescent membrane in a flow cell. A blue Led excites fluorescence from the membrane. Metal ions in the water flowing through the cell quench the fluorescence. The metals detected depend on the membrane composition. The flow cell is designed to be taken apart easily and the membrane replaced to detect other metals. The three colour photodiode allows detection of the fluorescence emitted at different wavelengths. Our instrument uses readily-available parts to reduce cost, allowing multiple instruments for rapid screening across a large area. The ion-selective fluorophores are Morin (2, 3,4,5,7 –pentahydroxy flavone, responds to AL(111) and tetraphenenylporporphyrin (responds to Zn(11). We report the sensitivity and selectivity of the instrument for these two metals. It is recommended that the device be adapted for use in pre-investigation of pollutions because the device is not limited to a particular membrane this allow for more fluorophore to be used, more so the wavelengths can be selectively filtered to suit its purpose.

## CLASSIFICATION OF APPLE VARIETIES ON THE BASIS OF VOLITILE ORGANICS BY SPME-GC-MS

Amanda J. Crook, Archana Tirmula, and Keyuri Patel
Chemistry
Faculty Research Advisor: Dr. Andrew Callendar

Various apple samples were analyzed for volatile organic components through solid-phase micro extraction gas chromatography mass spectrometry (SPME-GC-MS) to classify apple varieties. Samples were obtained from five different apple varieties commonly available in stores. Samples of apple flesh were obtained using a cork borer to ensure uniform size, shape and surface area. The SPME fiber injection technique was used to adsorb the volatile organic compounds (VOCs), which provide the distinctions between

flavors of apple varieties. SPME-GC-MS allowed only the VOCs of interest to be considered in this analysis, instead of the water, sugars, and other components of the apples. Variations in the VOCs upon oxidation were also observed to determine the effects of browning on apples. Principal components analysis (PCA) and a classification scheme were applied to the SPME-GC-MS data. Multiple classification schemes were tested and compared to determine the best method for classification. The application of PCA and the chosen classification scheme allowed the identities of unknown apples to be determined.

## PHYTOREMEDIATION OF PHARMACEUTICALS IN WATER USING DUCKWEED, BULRUSH AND PLANKTONIC ALGAE

Upul Deepthike
Chemistry
Faculty Research Advisors: Dr. Jeffrey Boles
Collaborator: Dr. Martha Wells, Center for the Management, Utilization and Protection of Water Resources

The occurrence of pharmaceuticals in water bodies is an emerging environmental concern. Even though the chronic effects of low-level exposure of these pharmaceuticals are not well-documented, s biologically active compounds they are potentially capable of interfereing with biological systems. In this research, the potential was assessed of using duckweed, bulrush and planktonic algae in pghytoremediation of several pharmaceuticals which are considered among the most harmful pharmaceuticals to aquatic environments   In addition, the accumulation of those pharmaceuticals in leaf and root parts of duckweed wa investigated. A combination of ultra hight performance liquird chromatography and ttime-of-flight mass spectrometry (UPLC-QTOF),  which provides the capability of fast and highly sensitive detection, were employed in the analysis.

## THEORETICAL STUDIES ON QUINONE REACTIVITY

Roshan Fernando
Chemistry
Faculty Research Advisor: Dr. Titus Albu

Quinones are a class of naturally occurring compounds that are biologically very relevant due to their ability to participate in redox couples. They act as electron carriers in the mitochondrion and act as electron acceptors in photosynthesis in both bacterial and higher plants. A theoretical study of a series of four benzoquinones (para-benzoquinone, ortho-benzoquinone, 2-chloro-para-benzoquinone, and 2-methyl-para-benzoquinone) was carried out using the mPWB95-44 density functional theory

with the 6-31+G(d,p) basis set.  One aspect of this study is focused in calculating redox potentials, and we identify nine relevant redox reactions.  The reversible potentials of all nine reactions and for all benzoquinone derivatives were determined, both in gas phase and aqueous phase. The results obtained are in very good agreement with experimental and previously published data.  Another aspect of the study is investigating the reactivity toward N-containing nucleophiles such as NH3, NH2CH3, and NHC2H5.  Transition states are investigating for the hydrogen abstraction process involve in the reactions.  Also we are investigating the reactivity of quinones with lysine (an amino acid).  The study will be later extended to other quinones and some other nucleophiles.

## MODIFIED SOLVENT SYSTEM FOR THE SIMULTANEOUS SOLVENT EXTRACTION OF CESIUM AND STRONTIUM

John Partridge
Chemistry
Faculty Research Advisor: Dr. Dale Ensor
Collaborators: Laetita Delmau, Bruce A. Moyer, and Dean Peterman

The effective simultaneous extraction of cesium and strontium from high level nuclear waste has received renewed interest as a result of the proposed recycling of civilian nuclear fuel.  Removal of the radionuclides of cesium and strontium, which initially account for the majority of radioactivity and heat production, from the waste would drastically reduce the amount of waste requiring long-term geologic storage, as well as reduce costs of building a recycling facility.  The extraction characteristics of 137Cs and 85Sr were studied using a variety of modifiers in the solvent. The effects of various solvent modifiers were measured as a function of concentrations of extractants, aqueous acidity, and third phase formation.  Experimental results indicate that a viable simultaneous extraction system for cesium and strontium from highly acidic waste can be developed.

## THEORETICAL MODELING OF ELECTRON TRANSFER BETWEEN CYTOCHROME C AND TRANSITION METAL COMPLEXES

Thusitha Pathirathne
Chemistry
Faculty Research Advisor: Dr. Scott H. Northrup

Electrostatic interactions have been identified as a key phenomenon that facilitates electron transfer reactions between proteins and their redox partners. Therefore, an accurate description of the electrostatic fields around a protein and its redox partner at various pH levels and salt concentrations is essential to analyze specific interactions

at the molecular level. The Poisson-Boltzmann equation has been widely used in conjunction with Brownian dynamics simulations to calculate diffusional association rate constants for electron transfer between redox partners. Previous work at TTU has correctly described protein electron transfer processes in terms of qualitative trends using this method, but has failed to provide a quantitatively accurate treatment of the ionic strength effects on the bimolecular rate constants. Taking this into account, in this work we enhanced the existing Brownian dynamics methodology developed extensively by Northrup and co-workers and the enhanced model is proved to be more robust as it models the electrostatic fields more accurately at various ionic strengths. Using the enhanced Brownian dynamics methodology we were able to quantitatively model the bimolecular kinetics of electron transfer between cytochrome c and seven different transition metal ion complexes, and extract intrinsic rate parameters governing the electron transfer event.

# CHEMISTRY
## UNDERGRADUATE STUDENTS

### SYNTHESIS AND CHARACTERIZATION OF NEW ACETYLPYRAZINE THIOSEMICARBAZONES

Michael Beck** and Keith Steelman
Chemistry
Faculty Research Advisor: Dr. Edward C. Lisic

Several new acetylpyrazine semicarbazone and thiosemicarbazone derivatives have been synthesized and characterized by melting point analysis, 1H NMR spectrometry and IR spectroscopy. These new compounds may have uses in medicinal chemistry, and will serve as ligands for the purpose of forming complexes with transition metals ions such as Cu(II) and Pd(II).

### CHEMICAL FINGERPRINTING OF CLANDESTINE METHAMPHETAMINE BY GC/MS/MS & LC/MS/MS TO ESTABLISH METH INDEX

Sarah C. Brinkley and Sri Bharat Madireddy
Chemistry
Faculty Research Advisor: Dr. Jeffrey O. Boles

Methamphetamine (N-methyl-1-phenylpropan-2-amine), a potent psycho-stimulant, has been a major cause of concern throughout the world, especially in the State of Tennessee.1 Illicit manufacture of methamphetamine in clandestine laboratories has been carried out with the minimal use of easily obtainable over-the-counter ingredients.1 Currently,

local law enforcement agencies lack the resources necessary to perform timely and cost effective investigation of meth-related crimes. However, research is currently being conducted to positively identify the 'chemical fingerprint' of seized clandestine methamphetamine; establishing a nationwide database containing such information would feasibly remedy this issue. This research focuses on developing an impurity profile for methamphetamine by LC/MS/MS; further supported by, both, qualitative and quantitative GC/MS/MS techniques. Selecting for specific markers - namely, ephedrine and benzylmethylketone (synthetic precursors), N-formylmethamphetamine (synthetic intermediate), and Caffeine (adulterant) - allows such a fingerprint to be constructed. An easily accessible directory, or METH INDEX, of confiscated methamphetamine becomes invaluable to officers of the law. The information this data-set provides will potentially create a unique advantage to criminal investigation, in that 1) drug-related crimes can be linked to clandestine chemists, providing the opportunity for more lengthy incarceration and 2) the methods utilized to synthesize methamphetamine, which evolve with the increasing restriction of starting materials, can be more rapidly determined.

**References**
1. United Nations, New York, Recommended methods for the identification and analysis of amphetamine, methamphetamine and their ring-substituted analogues in seized materials. ST/NAR/34 (2006)
2. C. J. Koester, B. D. Andresen, P. M. Grant, Optimum methamphetamine profiling with sample preparation by Solid-Phase Micro extraction. J. Forensic Sci. 47 (2002) 1002-1007

### ANALYSIS OF PRODUCT INHIBITION, STABILITY, AND CATION ACTIVATION OF ASPERGILLUS NIGER CELLULASE

Frank B. Couch, IV
Chemistry
Faculty Research Advisor: Dr. Jeffrey O. Boles

Our dependency on foreign oil can be reduced through the utilization of alternative fuels, such as cellulosic ethanol, which would also provide a fuel source more environmentally friendly than fossil fuels. The commercial availability of cellulosic ethanol is hampered at this time by the slow hydrolysis of cellulose. This project investigated 1) whether or not cellulase from A. niger suffers feedback (product) inhibition, 2) the stability of A. niger cellulase under varying temperature conditions, and 3) the effect of metal cations such as Na+, K+, Ca++, and Mg++ on specific activity. Feedback (product) inhibition was tested for by adding product (glucose) directly to the assay tubes. For 1, 2, and 5 µmol of glucose added, A. niger cellulase did not show

inhibition. Temperature stability was tested by incubating cellulase stock solutions for 24 hours at 50, 55, 60, 65, or 70 °C. A. niger cellulase showed a high degree of stability for 50, 55, and 60 °C, but rapidly lost activity at higher temperatures. Metal cations were added to the reaction mixture in various concentrations and the specific activity measured. Of the aforementioned ions, only Mg++ showed promise as an activator, while the others showed decreased activity or little change.

## THE PREPARATION OF 1-METHYL-3-OCTYLIMIDAZOLIUM CHLORIDE FOR USE AS A GREEN CHEMISTRY REACTION SOLVENT

Demiana Ghattas
Chemistry
Faculty Research Advisor: Dr. Dan Swartling

1-Methyl-3-octylimidazolium chloride has been prepared and will be used to replace volatile organic solvents in the synthetic procedures for selected compounds of interest.

## THE FORMULATION OF LOW-CARB LOW-FAT EGG-FREE DAIRY-FREE LIQUID NITROGEN ICE CREAMS

Aileen Guerrero and Demiana Ghattas
Chemistry
Faculty Research Advisor: Dr. Dan Swartling

For diabetics, people allergic to eggs and dairy products, and people wishing to reduce their calorie intake, the standard award-winning ice cream recipes are being reformulated to reduce carbohydrate content, reduce fat content, and eliminate egg and dairy products while still retaining the flavor and texture of the original recipe.

## SYNTHESIS AND CHARACTERIZATION OF A NEW SERIES OF PALLADIUM COMPOUNDS WITH WATER-SOLUBLE 5-FORMYL-2-FURAN THIOSEMICARBAZONE LIGANDS

Erik P. Hoy
Chemistry
Faculty Research Advisor: Dr. Edward C. Lisic

This work will present the synthesis of a new series of 5-formyl-2-furan sulfonic acid thiosemicarbazone compounds. A series of thiosemicarbazides (thiosemicarbazide, 4-methylthiosemicarbazide, 4-ethyl-3-thiosemicarbazide, 4-benzyl-3-thiosemicarbazide, 4-phenyl-3-thiosemicarbazide, 4,4-dimethyl-3-thiosemicarbazide) were combined with 5-formyl-2-furan sulfonic acid sodium salt to synthesize a new series of six new water-soluble ligands. These new compounds were characterized by 1H NMR. This work will also describe the synthesis of a new series of Pd(L)2 compounds, using potassium tetrachloropalladate(II), where L represents one of the six new ligands. The chelating thiosemicarbazone ligands bind to Pd in a bidentate fashion, not as tridentate ligands as might be expected.

## SYNTHESIS AND CHARACTERIZATION OF A NEW SERIES OF 5-ACETYL-URACIL THIOSEMICARBAZONE COMPOUNDS

Wesley Lisic and Michael Beck
Chemistry
Faculty Research Advisor: Dr. Edward C. Lisic

This work will present the synthesis of a new series of 5-Acetyl-Uracil thiosemicarbazone compounds. A series of thiosemicarbazides and semicarbazides (thiosemicarbazide, 4-methylthiosemicarbazide, 4-ethyl-3-thiosemicarbazide, 4-phenyl-3-thiosemicarbazide, 4-benzyl-3-thiosemicarbazide, 4-dimethyl-3-thiosemicarbazide, 4-phenylsemicarbazide hydrochloride, and semicarbazide hydrochloride) were combined with 5-Acetyl-Uracil to synthesize a new series of eight compounds. The new compounds were characterized via 1H NMR.

## ANALYSIS OF ORGANIC CONTAMINATION BY COAL MINING AND ASPHALT PRODUCTION

Jo Meagan Mansfield
Chemistry
Faculty Research Advisor: Dr. John Harwood
Collaborator: Mr. Gene Mullins

We have developed extraction and analysis methodologies for determination of organic contamination in samples taken from two areas affected by fossil fuel industries. Polynuclear aromatic hydrocarbons (PAHs) and other organic compounds from such operations can contaminate both the water and sediment of receiving streams. Our analysis steps include solid phase extraction and preconcentration of samples, and high-performance liquid chromatography /mass spectrometric analysis utilizing atmospheric pressure chemical ionization. The method provides a useful tool in monitoring streams with potential organic pollution created by coal mining, asphalt production, and other industrial activities. We will analyze samples from the segment of the Emory River which contains coal ash from the recent spill at the Kingston Coal Plant, and drainage from the Horseshoe Mountain coal mine site. We will present our analytical methodology, and results of our initial analyses of environmental samples.

## THE KNOEVENAGEL COUPLING OF MELDRUM'S ACID TO ALDEHYDES AND KETONES

Casey McCormick
Chemistry
Faculty Research Advisor: Dr. Dan Swartling

Meldrum's Acid is reacted with aldehydes and ketones to form the corresponding Knoevenagel adducts.  These will be used to prepare gamma amino acids.

## SYNTHESIS OF A SERIEW OF NAPTHAQUINON SULFONIC ACID THIOSEMICARBAZONE COMPUNDS AND USE IN FORMATION OF A SOLID SUPPORT SYSTEM

Megan Monteen and Kelly Monteen
Chemistry
Faculty Research Advisor: Dr. Edward C. Lisic

The synthesis and 1H NMR characterization of a series of 1,2-napthoquinone-4-sulfonic acid thiosemicarbazone (NQSA-TSC) ligands will be presented. These water-soluble ligands react with many different transition metal ions in aqueous solution to form highly colored complexes. The synthesis of some palladium complexes of these NQSA-TSC ligands will also be described, as well as their binding characteristics for analytical purposes on a solid support system.

## THE PREPARATION OF 1-BUTYL-3-METHYLMIDAZOLIUM BROMIDE FOR USE AS A GREEN CHEMISTRY REACTION SOLVENT

Sean Ochsenbein
Chemistry
Faculty Research Advisor: Dr. Dan Swartling

1-Butyl-3-methylmidazolium bromide has been prepared and will be used to replace volatile organic solvents in the synthetic procedures for selected compounds of interest.

## PRETREATMENT OF SWITCHGRASS FOR THE GLYCOSYL BIOCONVERSION TO CELLULOSIC ETHANOL

Jessika Pinto
Chemistry
Faculty Research Advisor: Dr. Jeffrey O. Boles

Cellulosic ethanol that originates from perennial grasses and municipal waste is an alternative fuel that can reduce our dependency on foreign oil while at the same time provide a more environmentally friendly fuel source. A large amount of municipal waste sorted for recycling is never recycled and ends up in landfills. Approximately 60% of municipal waste is organic and very high in cellulose content. Unfortunately, the commercial availability of cellulosic ethanol is plagued at this time by the slow hydrolysis of Cellulose (which produces the required sugar monomers necessary for bioconversion). This project investigates 1) the feasibility of various pre-treatment methodologies on several readily available and/or proposed feedstocks, and 2) the resultant yield in ethanol for each feedstock.

## ATTEMPTS AT MICHAEL ADDITION OF NITROMETHANE TO MELDRUM'S ACID ADDUCTS

Dan Roubik
Chemistry
Faculty Research Advisor: Dr. Dan Swartling

Nitromethane is added to adducts of Meldrum's acid with aldehydes and ketones to create nitromethyl products. These can be converted to the corresponding gamma amino acids in two additional steps.

## STUDY OF EFFECT OF SOLVENT POLARITY ON KINETICS OFHYDROLYSIS OF MICROMOLAR FERRIC IRON

Amy Sims
Chemistry
Faculty Research Advisor: Dr. Hong Zhang

Iron plays an important role in life and the environment.  We studied the effect of ethanol on Fe(III) hydrolysis kinetics using a redox analysis. A set of micromolar $FeCl_3$ solutions of a certain water:ethanol ratio (3:2, 2:2, 1:2) at pH 3.5 were prepared; at various time intervals, $NH_2OH \cdot HCl$ was added to reduce Fe(III) species to Fe(II), which was analyzed spectrophotometrically. UV-VIS spectrum was obtained for the $FeCl_3$ solution at each water:ethanol ratio. Ethanol did not change the general trend of the kinetics of Fe(II) concentration decrease, but increasing ethanol fraction

lowered initial Fe(II) concentrations and the rates of the Fe(II) decrease.  Ethanol did not change the general trend of change of the UV-Vis spectrum with time, but increasing ethanol fraction lowered the peak at ~300 nm. This study showed that varying solution polarity can be a useful means for studying the kinetics of Fe(III) hydrolysis and polymerization of hydroxy-Fe(III) species.

## GEOCACHING AS A WAY TO ENGAGE STUDENTS AND THE PUBLIC IN CHEMISTRY

Jenny Threet
Chemistry
Faculty Research Advisor: Dr. Dan Swartling

As a STEM activity incorporating GIS skills, math and chemistry skills, chemistry problems have been developed where the person has to use knowledge of chemical information to solve for the GPS coordinates of a location where something is hidden, then use a GPS receiver to find it. This provides the student with a fun way to engage the material presented in the problems.

# COMPUTER SCIENCE
## GRADUATE STUDENTS

### EXTENDING THE XEN HYPERVISOR TO CREATE A LIGHTWEIGHT AND ADAPTABLE HPC HYPERVISOR

Ferrol Aderholdt
Computer Science
Faculty Research Advisor: Dr. Ambareen Siraj
Collaborator: Dr. Stephen L. Scott,
Oak Ridge National Laboratory

In the field of High Performance Computing (HPC), currently there is a lot interest in virtualization.  Virtualization is the abstraction of hardware such that the execution environment is isolated into a virtual machine (VM). The VM is managed by a Virtual Machine Monitor (VMM), or hypervisor, that also ensures the underlying application binary interface (ABI). Virtualization presents many benefits as it allows more efficient usage of system resources and contains inherent fault tolerance with the ability to migrate virtual machines. The Xen hypervisor is a free and open source system that does not contain features like modularity and adaptability. This research presents two mechanisms that successfully enable Xen to become both lightweight and adaptable with general runtime tracing and profiling abilities. These mechanisms are the creation of Loadable Hypervisor Modules (LHMs) and the addition of

instrumentation capabilities that utilize LHMs. Incorporation of the mechanisms allow Xen to become more effective HPC hypervisor.

## PLAGIARISM DETECTION IN PROGRAMMING ASSIGNMENTS

Jeff Graves
Computer Science
Faculty Research Advisor: Dr. Bill Eberle

Plagiarism is a known issue in universities.  Students are often cautioned about the seriousness of plagiarism, but sometimes they choose to ignore these warnings.  The area of computer science has not escaped the problems of plagiarism among students.  It is not uncommon for students in introductory computer science courses to copy the source code of fellow students and submit it, with or without modifications, as their own work.  Detecting this type of plagiarism, sometimes termed collusion, can be difficult when large numbers of assignments are submitted. Detecting collusion would become much easier if one could be told which assignments were very similar in nature.  A promising area of research is in graph representation of source code.A graph-based approach could be used in an attempt to measure similarity in programming assignments. This research explores possible methods of converting source code files into graphs, along with how graph theory can be applied to measure similarity in source code graphs. Experiments will be performed on assignments submitted for undergraduate courses in computer science where known instances of plagiarism occurred.

## DISCOVERING KNOWLEDGE FRONTIERS IN HIERARCHICAL CLUSTER TREES

Matt Honeycutt
Computer Science
Faculty Research Advisor: Dr. Doug Talbert

Hierarchical clustering is an unsupervised learning technique for exploratory data analysis.  Unlike traditional, flat clustering clusterers, hierarchical clusterers allow the user to explore the data at various levels of abstraction. Classification is a supervised learning technique that attempts to discovery rules or other predictive models that can correctly assign predefined labels to previously unseen objects.  By combining a hierarchical cluster tree with performance statistics from a classifier, Knowledge Frontier Discovery identifies meaningful subpopulations on which a classifier has similar predictive performance.  These discovered knowledge frontiers are subpopulations of the data where any sub-partition with a significantly different predictive accuracy is not meaningful.  The Knowledge Frontier Discovery process incorporates ideas from many areas of machine learning research including clustering

and top-down induction of decision trees. A user-specified parameter guides the discovery process and enables the tool to find frontiers that are at the desired level of specificity.

## FPGA-BASED
## FUZZY INTRUSION DETECTION SYSTEM

Marbin Pazos-Revilla
Computer Science
Faculty Research Advisor: Dr. Ambareen Siraj

The costs associated with the disruption of crucial network services, and the damages caused by malicious attacks can be devastating to any organization. To prevent and mitigate these attacks considerable amounts of resources are used in deploying devices like Intrusion Detection Systems (IDS). IDSs act as security watch dogs and report security violations resulting from attacks. Although they have been proven useful, the inherent nature of conventional rule-based IDSs and the trends in bandwidth growth, among other factors, still provide loopholes allowing attacks to fall through cracks and remain outside radar. This research presents a novel approach integrating Field Programmable Gate Arrays (FPGA) and Fuzzy Logic in the field of network intrusion detection. The FPGA-based Fuzzy IDS addresses the aforementioned issues in conventional rule-based IDSs and have the potential to provide high throughput, parallelism, low non-recurring engineering costs, and the capability of inexact reasoning with its embedded Fuzzy Inference Engine - characteristics that makes it unique from current IDS approaches.

## COMPUTER SCIENCE
## UNDERGRADUATE STUDENTS

## USING KEYLOGGER
## FOR INSIDER THREAT DETECTION

Matt Gibbs
Computer Science
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Insider threat is still one of the biggest threats to a company where sensitive information is compromised by its own employees. Although infamous for its malicious uses, keylogging software can be effectively utilized by companies to monitor their employees' activities for possible security violations. Keylogger software can capture and monitor keystrokes and mouse clicks and log them for analysis. The primary focus of this research is to build keylogger monitoring software to collect and keep employee records for analysis of insider threats. Running a keylogger as a service in the background can enable the program to collect data from keystrokes without any visible intervention with employees' daily work. In a company network, each workstation can be installed with the monitoring software,

and all keystrokes and other data it collects can be sent to a central location. This data can then be analyzed by system administrators to collect information on employees' activities during company time.

## EARTH SCIENCES
## AND GEOLOGY
## GRADUATE STUDENTS

## ENVIRONMENTAL IMPACT OF CLANDESTINE
## METHAMPHETAMINE LABORATORIES

Tammy Boles
Environmental Sciences-Chemistry
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Utilization and Protection of Water Resources

Methamphetamine is a highly addictive, powerful nervous system stimulant. Because methamphetamine is so addictive, it is illegal to manufacture or use the drug without a prescription under Federal Law. Clandestine laboratories have proliferated and have been found in all states of the United States because methamphetamine is cheap and easily produced. Although harmful chemicals from the production of methamphetamine are released into the air, soil, and water, relatively few studies have been performed to determine the effect of the chemicals on the environment. Data from studies that have been performed show methamphetamine present in influent and effluent from wastewater treatment plants in the United States and Europe, as well as in some surface waters in Europe. For this proposed research, water samples from the local waste water treatment plant and from sewer pipes near known clandestine laboratories, and soil samples from areas around clandestine dump sites will be analyzed for methamphetamine, its precursors, by-products and degradates by liquid chromatography-tandem mass spectrometry. Remediation of illegal laboratory sites will also be investigated.

## DEVELOPMENT AND TESTING
## OF ADAPTIVE CLUSTER SAMPLING DESIGNS
## FOR DUSKYTAIL DARTERS

Johnathan G. Davis
Environmental Sciences-Biology
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Collaborator: Dr. David Smith,
Department of Biology; Department of Mathematics

The duskytail darter Etheostoma percnurum is an endangered species in Tennessee in need of conservation

due to declines in population size and habitat loss. The goal of this study was to develop, simulate, and test adaptive cluster sampling (ACS) designs to construct a cost-effective monitoring program that detects changes in and estimates population size. ACS designs have effectively sampled

various rare and endangered species and may be applicable to habitat-specific stream fishes. Baseline distributional data was collected at three sites on the Big South Fork River and was used in computer simulation of multiple ACS designs. Simulations resampled baseline data from each site to estimate population size, mean units sampled, and mean squared error. Designs that performed well were field tested at 15 sites to estimate population size and sampling effort. ACS designs with a high stopping rule and low condition factor had lower error, but required large sampling effort and were not cost-effective. ACS designs were applied successfully to sample duskytail darters and estimate population size. They can be an alternative design for biologists to use to monitor rare or endangered stream fishes. Further testing is required to find a balance between sampling effort and error.

## IDENTIFICATION OF EICOSANOIDS IN FISH TISSUES

Alisha Pendergrass
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Department of Chemistry;  Center for the Management, Utilization and Protection of Water Resources

The endocrine system is a chemical communication process which regulates internal operations including reproduction. Endocrine-disrupting compounds (EDCs) mimic natural hormones and interfere with the internal signaling and regulatory systems of an organism. EDCs can enter the environment through various waste products. The intersex condition (having signs of ovotestis) is considered to be a biological indicator of reproductive endocrine disruption in a number of fish species. Eicosanoids are endogenous chemicals derived from fatty acids and are found in many animal tissues. Eicosanoids are involved in physiological processes including reproductive function. The objectives of this research were to: 1) effectively extract eicosanoids and other endogenous chemicals from fish samples for chromatographic analysis, 2) compile chromatographic data to obtain the chemical profiles for the fish sampled, and 3) determine if there are differences in the chemical profiles to evaluate if eicosanoids and other endogenous chemicals are significant indicators of the fish intersex condition. Chromatographic analyses were conducted on the Waters Aquity Ultra Performance Liquid Chromatograph Mass Spectrometer Quadrupole Time of Flight (UPLC MS-MS Q-TOF) Premier instrument. Identification of eicosanoids

from mass spectra produced fish profiles which could aid evaluation of the fish intersex condition which can be indicative of water pollution.

## INFLUENCE OF DISSOLVED ORGANIC MATTER ON POTABLE WATER PRODUCTION

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Safe drinking water is a necessity in our daily lives. Disinfection of water reduces waterborne diseases, but concomitantly, disinfection by-products (DBP) are formed in finished drinking water by the reaction of natural organic matter (NOM), present in raw water, with disinfectants used in this process. Regulated by the U.S. Environmental Protection Agency, DBPs of major concern include trihalomethanes (THMs) and haloacetic acids (HAAs), because these compounds are suspected of causing diverse types of cancers and adverse birth outcomes. Typical parameters used as surrogates of organic matter, i.e. DBP precursors, in water include total organic carbon (TOC), dissolved organic carbon (DOC), ultraviolet absorbance (UV) at 254 nm, and specific ultraviolet absorbance (SUVA). Fluorescence spectroscopy is not commonly used as a surrogate for indicating the presence of DBP precursors, but it has the potential to be used for this purpose. In this research, three-dimensional fluorescence spectroscopy or excitation-emission matrix (EEM) spectroscopy is used to generate maps on which specific spectral signatures of NOM fluorophores can be localized. The primary objective in this research is to observe if a relationship exists among surrogates of natural organic matter in drinking water. Water from different sources and seasons were collected and analyzed.

# EARTH SCIENCES
## UNDERGRADUATE STUDENTS

## EROSION AND SEDIMENT TRANSPORT IN A SMALL URBAN WATERSHED

Douglas Oyston
Earth Sciences
Faculty Research Advisor: Dr. Evan Hart

Transport of suspended sediment plays a significant role in estimating drainage basins sediment budget. A sediment budget is a quantitative statement of the rates of production, transport, and discharge of detritus (Dietrich et al., 1990). Suspended sediment also plays a key role in

transporting contaminants in a river, and can affect the aquatic life of its ecosystem. Measuring sediment erosion and transport in all parts of a watershed is impossible. This research aims to estimate the erosion and sediment transport in an urbanized watershed based on erosion pin measurements, suspended sediment sampling of stream flow, and surveys of stream channels. Erosion pins placed in the watershed 5 years ago by previous students were re-surveyed. Channel cross-sections were also re-surveyed. Suspended sediment sampling was done during flood and low flow periods. Results suggest that sinkholes and caves in the watershed play an important role in regulating the amount of sediment transported downstream. Erosion pins and channel cross-section surveys show that erosion of uplands and streams is active. These results have important implications for downstream water quality.

# PHYSICS
## UNDERGRADUATE STUDENTS

### SIMULATION OF VELOCITY FILTERS IN THE DARESBURY RECOIL SEPARATOR AT THE HRIBF

J. P. Rogers
Physics
Faculty Research Advisor: Dr. R. L. Kozub
Collaborators: S. D. Pain, M. S. Smith, D. W. Bardayan, and Y. Liu, Oak Ridge National Laboratory; M. Matos, LSU

The Daresbury Recoil Separator (DRS) at Oak Ridge National Lab's (ORNL) Holifield Radioactive Ion Beam Facility (HRIBF) is used for the study of nuclear reactions of astrophysical importance. For example, the DRS enables direct measurements of proton capture reactions on radioactive ions which occur in stellar explosions such as novae and X-ray bursts. The DRS uses velocity filters (Wien filters) that are tuned to transmit the reaction products with a specific velocity while deflecting the unreacted primary beam particles away from the optical axis, where they are stopped on adjustable slits. Data from earlier calculations of the electromagnetic fields inside and around the filters has been implemented into a FORTRAN program to provide accurate calculations and graphic representations of particle trajectories through the Wien filters. This information can be used to predetermine optimum positions of the slits for future experiments. The program will be used as an experimental setup tool for the DRS.

# COUNSELING AND PSYCHOLOGY
## UNDERGRADUATE STUDENTS

### INTERNET PORNOGRAPHY USE BY COLLEGE STUDENTS

Zach Ludwig
Counseling and Psychology
Faculty Research Advisor: Dr. Matthew Zagumny

My research, to be present in poster form, intends to evaluate and record attitudes about Internet pornography held by college students, motivations for exploring sexually explicit material online, and consequences experienced by this group in offline activities. This study utilized an online questionnaire that has been completed by more than two hundred college students, to assess Internet pornography use. A multiple correlation regression analysis will be implemented to determine if there is a correlation between a number of factors including, if attitudes about, reasons for, and amount of time spent viewing sexually explicit material online results in offline repercussions.

### ATTRACTIVENESS AND NUMBER OF SEXUAL PARTNERS: ATTRIBUTIONS OF SELF-ESTEEM, COMMITMENT, AND RELIGIOSITY

Annette Lynch
Counseling and Psychology
Faculty Research Advisor: Dr. Linda Giesbrecht-Bettoli

This study examined the effects of physical attractiveness and the number of sexual partners on 6-point Likert-type scales of perceived self-esteem, commitment, and religiosity in an undergraduate sample of 240. Participants were shown pictures of either an attractive or unattractive female or males and provided with information regarding the number of previous sexual partners. A 2(Gender of Subjects)X 2( Attractiveness)X 2(Number of Sexual Partners) X 3(Self-Esteem/Commitment/Religiosity) was evaluated. Participants provided both objective and self-ratings of self esteem, commitment and religiosity. In addition, three multiple regressions were performed.

## OBJECTIFICATION OF MALES IN THE MEDIA: DRIVE FOR MUSCULARITY AND BODY SATISFACTION

Brandie Nichole Storm-Rich Counseling and Psychology
Faculty Research Advisor: Dr. Linda Giesbrecht-Bettoli

The current study examined body satisfaction in men pertaining to their drive for muscularity, sexual orientation, media viewing habits, and ethnicity. The Male Body Attitudes Scale was used to assess participants' overall body satisfaction. A Sociocultural Attitudes Toward Appearance Scale was used to measure pressures associated with the media. The participants completed the Drive for Muscularity Scale to determine their attitudes toward increasing muscularity. Participants were also asked questions pertaining to their sexual preference, media viewing habits, and ethnicity. A multiple regression analysis was performed using sexual orientation, race, media exposure, sociocultural attitudes toward appearance, and drive for muscularity to predict overall body satisfaction. Both drive for muscularity and sociocultural attitudes toward appearance were found to be significant predictors of overall body satisfaction.

## KNOWING WHEN TO FOLD'EM: PREDICTORS OF POKER STRATEGY

Jonathan Wood
Counseling and Psychology
Faculty Research Advisor: Dr. Zachary Wilcox

The current study examined predictors of the frequency of raising as well as the frequency of self-reported bluffing behavior In Texas Hold'em poker. It was hypothesized that perceived skill level (PSL), participants' sex, and level of egocentrism would be predictors of the frequency of raising. It was also hypothesized that PSL, participants' sex, level of egocentrism, and frequency of raising would be predictors of the frequency of bluffing. Results showed that sex and PSL are predictive of raising, and that sex and raising are predictive of self-reported bluffing. While the results suggest that women and beginners are more likely to raise and that women and those who raise are more likely to be bluffing, it is suggested that other factors not measured in the current study may influence such decision-making behavior in a more real-world environment.

## CURRICULUM AND INSTRUCTION
### GRADUATE STUDENTS

## CHALLENGING BEHAVIOR: IMPACT OF TEACHER BELIEFS ON PRACTICE

Martha Howard
Curriculum & Instruction
Faculty Research Advisor: Dr. Lisa Zagumny

This research uncovers the relationship between teacher beliefs about child discipline and the consequent practice within their preschool classroom setting. Three state licensed child care providers within the Upper Cumberland area of Tennessee were interviewed and observed in their child care setting to determine if their practice is impacted by their personal beliefs related to discipline and the occurrence of challenging behavior. Documents, interviews, and observations have been analyzed in an effort to uncover useful resources or potential resources that might be an impetus for change within the early childhood profession.

## EXCEPTIONAL LEARNING
### ?????? STUDENTS

## WHAT IS READING?: AN INTERPRETIVE STUDY OF ADOLESCENT READING CONSTRUCTIONS

Julie C. Baker
Exceptional Learning, Literacy
Faculty Research Advisor: Dr. Lisa Zagumny

In adolescent literacy research, there is a gap in literature relating to adolescents' constructions of reading. It is not possible to gather significant research on the topic without hearing from the adolescents themselves. In this interpretive study using a case study approach, three adolescent participants were interviewed and one high school reading class was observed. The adolescents attended three different public, urban secondary schools. The purpose of the study is to discover what these three adolescents consider to be "reading" and how they construct what reading means to them. The primary research question is What is reading to adolescents? Answers to these questions may shed light on adolescent beliefs about, motivations for, attitudes toward, and connections to reading. By making these connections to adolescents concerning their constructions of reading, changes may be proposed for future research to promote reading, reading awareness, and reading success for adolescent readers. Through careful examination and interpretation of the interviews, observations, and document analyses, we will better understand how reading is constructed in the minds of adolescents and be better equipped to answer these important research questions.

# CHEMICAL ENGINEERING
## GRADUATE STUDENTS

### UNDERSTANDING CAPACITY FADE PREDICTION OF LITHIUM ION BATTERIES

Mounika Arabandi
Chemical Engineering
Faculty Research Advisors: Dr. Venkat R. Subramanian
Collaborator: Dr. Vijayasekaran Boovaragavan

Lithium-ion batteries are currently one of the most popular types of battery for portable electronics, which are being used for consumer electronics, defense, automotive, and aerospace applications. The battery loses its capacity to hold and deliver the energy when the number of cycle increases. Therefore it is essential to quantify the capacity loss for a given cycling protocol. These losses are mainly due to the variations in the transport and kinetic parameters caused by the reduced pore volume in the porous electrodes. A model that updates transport and kinetic parameters as a function of cycle number is developed. The unknown parameters that were estimated are the solid-phase diffusion coefficient Dsn and the reaction rate Kn in the negative electrode. These model parameters reduced monotonically with cycle number, which is consistent with a monotonic decrease in the pore volume in the negative electrode.

### ANTIOXIDANTS AS OXYGEN RADICAL SCAVENGERS IN FUEL CELL SYSTEMS

Daniel Betancourt
Chemical Engineering
Faculty Research Advisor: Dr. Cynthia A. Rice-York

Oxygen radicals have been shown to be a major source of degradation to Polymer Electrolyte Membrane Fuel Cell (PEMFC) components. They have been shown to be especially damaging to Nafion™ membranes. Fuel Cell (FC) degradation issues are especially relevant and complex since they are interconnected, such that the degradation of one material initiates or accelerates degradation of others. Innovation of FC materials in response to radical attacks up until this point has involved designing alternate membranes, with functional groups that are not susceptible to radical reactions or increasing membrane thickness. These alternate membranes have not, however, been capable of successfully replicating the high proton conductivity of Nafion™. On the other hand, increasing membrane thickness increases the materials cost of the FC, which is already too high. Biological beings also suffer from the presence of radicals; these radicals can have devastating effects on living systems, for example, oxygen radicals in the human body have been shown to greatly enhance the presence of malignant tumors. These systems have adopted antioxidants as part of the solution. My proposal uses the wisdom of evolution by studying the possibility of incorporating antioxidants to FC systems.

### SURVEY OF COMMERCIAL CARBON SUPPORTED PLATINUM CATALYSTS: DURABILITY STUDIES FOR AUTOMOTIVE APPLICATIONS

Daniel Betancourt
Chemical Engineering
Faculty Research Advisor: Dr. Cynthia A. Rice-York

Polymer Electrolyte Membrane Fuel Cells (PEMFCs) show promise as being a potential part of the solution for the current energy crisis as well as offering an environmentally benign alternative to the combustion engine. Introduction of PEMFCs however, has not been successful because of two main shortcomings: high cost and poor durability. To this end, this project will explore some of the catalyst durability issues and seek to give a better measure and relation to predict durability. Currently, there are studies that relate catalyst size, distribution and carbon support to their durability. These studies are not comparable, however, since they use accelerated durability test protocols which have differing effects on different catalyst types. Additionally, variations in catalyst preparation procedures have not been studied as a source of variation of performance. This study seeks to cohesively link the catalyst activity to its durability. Experimental techniques include Cyclic Voltammetry and Oxygen Reduction Reaction with a Rotating Disk Electrode to assess surface area and activity respectively. A survey of the commercially available carbon supported catalysts will be conducted; the work will provide greater insight into durability issues and will produce better information for Fuel Cell manufacturers, ultimately providing design criteria for more active/durable catalysts.

### FACTORS AFFECTING NANOPARTICLE DISPERSION

Deepika R. Gollamandala
Chemical Engineering
Faculty Research Advisor: Dr. Ileana C. Carpen.

Addition of nanosized particles to a polymer solution/matrix can lead to new and improved properties over conventional composites using larger filler particles. In this work, we investigated systems of nanoparticles and polymer using Brownian dynamic simulations. The shape of the nanoparticles was considered to be spherical and the polymer architecture was modeled as bead rod chains. The degree of dispersion and agglomeration in the system were characterized by mean square displacement. The effects of various individual factors, including nanoparticle polymer

interactions, polymer chain length, and relative volume fractions, on the dispersion of nanoparticles in the polymer matrix were analyzed and presented.

## TWO-PHASE FLOW: BUOYANCY DRIVEN FLOW OF A PARTIALLY MISCIBLE DROPLET AT LOW REYNOLDS NUMBER

Manohar Gottapu
Chemical Engineering
Faculty Research Advisor: Dr. Ileana C. Carpen

Mass transfer between droplets and a surrounding fluid is of central importance in many industrial processes such as liquid extraction and the aeration of bioreactors. In the low Reynolds number regime (Re<<1), the buoyancy-driven motion of a droplet in a partially miscible high viscosity fluid is accompanied by compositional gradients and is found to be qualitatively different from the classical motion of an immiscible droplet as given by the Hadamard-Rybczynski [20, 42] solution. Previous experimental studies have shown that a 'puddle' region develops on the downstream side of the drop due to convective-diffusive flows [4, 16]. In this work, we examine a single spherical droplet partially miscible with an infinite fluid phase and present an analysis that takes into account the partial miscibility of the drop with the ambient fluid. We qualitatively compare the predictions of this study with previous experimental results.

## KINETICS OF FAST PYROLYSIS OF EXPANDABLE POLYSTYRENE (EPS)

Pravin Kannan
Chemical Engineering
Faculty Research Advisors: Dr. Joseph J. Biernacki
and Dr. Donald P. Visco, Jr.

Fast pyrolysis technique offers a convenient way to investigate decomposition kinetics of various hydrocarbon based substances, including plastics and bio mass. Fast pyrolysis techniques minimize the influence of mass and heat transfer limitations often encountered in thermal analysis techniques, including combined thermogravimetry-mass spectroscopy (TG-MS) instruments and thus provide relatively better intrinsic kinetic information. In this study, a simple laboratory scale fast pyrolysis technique have been developed and demonstrated for the study of EPS decomposition kinetics. Pyrolysis experiments were performed at different experimental conditions of temperature and gaseous environment. The cumulative gaseous yield were determined using a flame ionization detector (FID) connected in series with the reactor. The governing equations for a tubular reactor type were modified and applied appropriately to obtain kinetic parameters, including activation energy and rate constant for the EPS decomposition process.

## USING PULSED CORONA DISCHARGES TO ELIMINATE POLLUTANTS FROM DRINKINIG WATER OR FLUIDS: A RESEARCH PROPOSAL

Chinyere P. Mbachu
Chemical Engineering
Faculty Research Advisor: Dr. Pedro E. Arce

The use of high oxidation methods to eliminate contaminants from drinking water or fluids is an attractive and efficient approach. Earlier work (Sharma et al., 1993) has shown the elimination of highly toxic contaminants such as phenol and more recently fumic traces (Smith, 2004) and proteins from water fluents (Ibañez, 2004). Pulsed corona high oxidation can be enhanced by adding either oxygen, in order to produce high active radicals, or iron to increase the effectiveness by the presence of the photo-Fenton reaction. In this research proposal, we are interesting in determining the efficiency of the method in application such as sanitation of drinking water or other related fluids such as fruit juices. In particular, the technique has a low heat generation and leads to negligible or moderated temperature increases. This option is highly desirable as an alternative to high temperature methods such as pasteurization. Both organic and biological contaminants will be tested experimentally to determinate the ability of pulsed corona in eliminating them and leading to a safe drinking product.

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## DUAL-ION CONDUCTING MEMBRANES FOR PORTABLE POWER FUEL CELLS

Rajavardhan Reddy Nagolu
Chemical Engineering
Faculty Research Advisor: Dr. Cynthia Ann Rice-York

Portable Power for military applications require high power density liquid fuel cells operating around 250°C. One candidate is Direct Methanol Fuel Cells(DMFC) with a dual ion conductor. The ionic conductivity of $Sn_{0.9}In_{0.1}P_2O_7$ ceramic was investigated under various atmospheres within the temperature range of 130-230°C. The $Sn_{0.9}In_{0.1}P_2O_7$ can conduct both protons and oxide ions at low temperatures (130-230°C). This ceramic provides $O_2-$ to anode to facilitate complete oxidation of reaction intermediates. However, $Sn_{0.9}In_{0.1}P_2O_7$ suffers from low proton conductivity. To improve the proton conductivity it is desirable to form a composite membrane with a high

proton conducting membrane. The performance of DMFC with Sn0.9In0.1P2O7-Nafion composite membranes was stable up to 120°C exhibited dual ion conductivity. We are looking for alternative composite membranes combine with Sn0.9In0.1P2O7 to improve the ionic conductivity at elevated temperatures.

## COLLOIDAL MODELS: GOLD NANOPARTICLE INTERACTIONS WITH HUMIC SUBSTANCES

Vasanta L. Pallem
Chemical Engineering
Faculty Research Advisors: Dr. Holly A. Stretz
and Dr. Martha J. M. Wells
Department of Chemical Engineering, Center for the Management, Utilization, and Protection of Water Resources and Department of Chemistry

The interaction of biomedical imaging gold nanoparticles with environmental entities such as humic substances was investigated applying dynamic light scattering. The increasing applications of gold nanoparticles in biomedical imaging and cancer therapy indicate potential for their subsequent release into surface waters. Therefore, it is primarily important to understand the interactions of gold nanoparticles with natural organic matter (humic substances), which will play a major role in the fate and transport of these particles in aquatic systems. The current study investigates the size changes and zeta potential variations taking place on gold nanoparticles coated with citrate, due to interactions with commercial humic acid (HA), having concentrations of 2 and 8 ppm. Different colloidal models for the interactions between gold nanoparticles and humic acids are also presented. The models are useful to potentially design environmentally safe strategies in the use and application of gold nanoparticles in a variety of novel technologies.

## DIAGNOSTIC GOLD NANOPARTICLES: INTERACTIONS WITH HUMIC SUBSTANCES

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Gold nanoparticles have potential applications in drug delivery, biomedical imaging and chemical sensing (1-3); however, their fate and transport in the environment is relatively unknown. The interactions of gold nanoparticles with environmental entities like humic substances present in natural aquatic systems play a vital role in their fate and transformation. In this respect, it is vital

to understand any chemical or photo-physical changes caused due to the interactions between nanoparticles and humic substances, which can provide insight into the aggregation behavior of these nanoparticles. This doctoral study is aimed at understanding the dispersability behavior of gold nanoparticles in surface waters in order to prevent potentially damaging effects in the environment. The interactions of humic substances with gold nanoparticles coated with two different surfactants β-D-glucose and citrate was investigated applying UV-Vis absorbance and fluorescence spectroscopy. Humic substances (HS) are fluorescent in nature, providing an interesting tool to characterize the interaction between these natural polyelectrolytes and model water soluble gold nanoparticles. Quenching of fluorescence intensity was observed with β-D-glucose coated gold nanoparticles whereas an enhancement effect was noticed with the citrate coated particles. Examining the quenching/ enhancement of fluorescence provides insight into the structural changes taking place at the gold nanoparticle and humic acid interface. Knowledge of the interactions between humic substances and gold nanoparticles will enable development of environmentally safe gold nanoparticles.

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## AN ELECTROKINETIC-HYDRODYNAMICS-EKHD BASED APPROACH TO DETERMINE EFFECTIVE TRANSPORT PARAMETERS: ILLUSTRATIVE RESULTS AND COMPARISON

Jennifer A. Pascal
Chemical Engineering
Faculty Research Advisor: Dr. Pedro E. Arce
Collaborator: Dr. Mario A. Oyanader

A number of contributions have been made to the field of electrokinetics, i.e. electrophoresis, electroosmosis, etc. as it relates to the behavior of diffusion and hydrodynamics in various systems. Many of these efforts have been influenced by the work conducted by the group of Giddings (see, for example, Martin and Giddings [1], [2]) who worked in the area of field flow fractionation (FFF). In this separation technique, an orthogonal applied field (i.e. gravitational, electrical, etc.) drives the motion of the molecules towards the channel walls. Among illustrative contributions and without being thorough in the literature citations, Giddings ([1]), based on nonequilibrium theory, predicted retention

times in various types of FFF devices. Brenner and Edwards ([3]), examined a Couette-based flow apparatus with cross flow in which equations governing the transport of Brownian solute particles (i.e. diffusivity and velocity) were developed. A powerful mathematical framework that is currently available ([6]) for these types of problems is the coupling of EKHD with the spatial averaging method ([4], [5], [6], [7], [8]). In this presentation, the authors will present illustrative results for Couette hydrodynamic flows (i.e. optimal separation times) obtained using EKHD and compare these predictions with results found in the literature.

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## ELECTROKINETIC-HYDRODYNAMICS (EKHD): AN EFFICIENT FRAMEWORK FOR SYSTEMATIC RESEARCH

Jennifer A. Pascal
Chemical Engineering
Faculty Research Advisor: Dr. Pedro E. Arce
Collaborator: Dr. Mario A. Oyanader

Currently there are many problems in Chemical Engineering that involve the application of an applied electrical field to a fibrous or porous media in a variety of relevant technological processes. Examples of these types of problems are the separation of biomacromolecules, such as proteins and DNA, bioremediation, drug delivery, and coating flows, among others. These types of problems can be described by the fundamentals of "electrokinetic-hydrodynamics" or EKHD, for short. What makes the applications within the domain of electrokinetic-hydrodynamics unique is that unlike electrochemical systems, bulk motion of the fluid occurs. Therefore, we can view EKHD as involving two domains: the motion of the fluid (electrohydrodynamics) and the motion of the solute/analyte (electro and convective-diffusive transport). It is apparent that these two domains are representative of two different scales, the continuum (fluid) and the discrete (solute). This contribution will discuss how EKHD is an efficient framework for the investigation of systems with low and high values of applied electrical fields.

## TOWARDS OPTIMAL DESIGN OF LITHIUM ION BATTERIES

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Faculty Research Advisor: Dr. Venkat Subramanian
Collaborator: Dr. Vijayasekaran Boovaragavan

Lithium-ion battery chemistry has been identified as a good candidate for high-power/high-energy secondary batteries. Applications for batteries range from implantable cardiovascular defibrillators (ICDs) operating at 10 µA current to hybrid vehicles requiring pulses of 100 A. While physics-based models have been widely developed and studied for these systems, these models have not been employed for dynamic optimization of operating conditions or for designing electrodes for a specific performance objective. Macroscopic models have been applied to optimize the electrode thickness or porosity. These studies have been performed by comparing the Ragone plots for different design parameters. This work focuses on the application of first-principles models to the global optimization of multiple battery design parameters. The model will be used for simultaneous optimization of the applied current density (I), porosity ($\varepsilon$) and thicknesses of the separator and the two electrodes (Is, In, Ip). Optimal values of these parameters incorporated in designing batteries ensure lower cost and higher efficiency of the battery, and also improves the cycle life of the battery.

## ROLE OF BOTH ORTHOGONAL AND AXIAL ELECTRICAL FIELDS IN ELECTROPHORESIS: SOME COMPARATIVE OBSERVATIONS

Hope Sedrick
Chemical Engineering
Faculty Research Advisor: Dr. Pedro Arce
Collaborator: Dr. Mario Oyanader

When using electrical fields to separate molecular species for example pharmaceutical applications, a researcher must know an approximate optimal separation time for the two molecules. In order to calculate this optimal separation time, one must look at the contributions of the varying applied electrical fields. In this study, we analyze the effect, on optimal time of separations, of different types of applied electrical fields, i.e. orthogonal, parallel and in both directions for a typical case of a capillary with Poiseuille flow and no EOF. The case for the no applied electrical field will be also included for comparison purposes. Future work could include the comparison of these four cases for different convective regimes such as Couette or/and electroosmotic flow.

## EFFECT OF CHANNEL MORPHOLOGY ON ELECTROPHORESIS OF BIO-MOLECULES: PRELIMINARY INVESTIGATION

Jyothirmai J. Simhadri
Chemical Engineering
Faculty Research Advisor: Dr. Pedro E. Arce
Collaborators: Dr. Mario O. Oyanader and Dr. Holly A. Stretz

Electrophoresis in polymer hydrogels with nanometer-scale pore structure are widely used for the separation and purification of biological macromolecules. In gel-electrophoresis, the internal morphology of the gel also plays an important role in improving the separation. Tuning the nanometer-scale pore structure of the gel either by templating or by adding nanoparticles to improve separations has been the current area of focus. Moreover, analysis of the effects of the nature of the pore alignment, pore length and diameters on the transport of macromolecules is an important aspect to be studied either analytically or computationally as shown by previous efforts (Trinh et al, 1999; Hidalgo et. al, 2007). In this research we propose to computationally analyze different pore models and study the effect of geometry on the transport of biomolecules in this anisotropic-like media.

**References:**
1. Trinh, S., B.R. Locke and P.E. Arce, "Convective and Electroconvective Transport in Non-Uniform Channels with Application to Macromolecular Separations," Separation and Purification Technology, 15, 255 (1999).
2. Hidalgo, R., M. A. Oyanader (*), and P. E. Arce, "Dispersive Mixing Effect Caused by Combined Effect of Channel Morphology and Electrophoretic Mobility in Poiseuille Flows." AIChE Annual Meeting, Salt Lake City, 2007. (*) Speaker.

## ELECTROPHORESIS OF BIO-MOLECULES IN A DIVERGING CHANNEL: COMPARISON OF COMPUTATIONAL AND ANALYTICAL RESULTS

Jyothirmai J. Simhadri and Jennifer A. Pascal
Chemical Engineering
Faculty Research Advisor: Dr. Pedro E. Arce
Collaborators: Dr. Mario Oyanader and Dr. Holly A. Stretz

Research involving polymer gels with embedded nanoparticles of varying properties is quite attractive because of the multitude of potential applications, including separation of biomacromolecules, tissue scaffold growth, as well as the analysis of the efficiency and control of drug delivery. In gel-electrophoresis, the internal morphology of the gel also plays an important role in improving the separation. Tuning the nanometer-scale pore structure of the gel either by templating or by adding nanoparticles

to improve separations has been the current area of focus. Moreover, the analysis of the effects of the nature of the pore alignment, pore length and diameters on the transport of macromolecules are important aspects to be studied either analytically or computationally as shown by previous efforts (Trinh et al, 1999; Hidalgo et. al, 2007) In this presentation we will compare computational results obtained from the analysis of electrophoresis in a diverging channel to those obtained analytically based on the use of EKHD approaches (Pascal et al., 2008).

**References:**
1. Trinh, S., B.R. Locke and P.E. Arce, "Convective and Electroconvective Transport in Non-Uniform Channels with Application to Macromolecular Separations," Separation and Purification Technology, 15, 255 (1999).
2. Hidalgo, R., M. A. Oyanader (*), and P. E. Arce, "Dispersive Mixing Effect Caused by Combined Effect of Channel Morphology and Electrophoretic Mobility in Poiseuille Flows." AIChE Annual Meeting, Salt Lake City, 2007. (*) Speaker.
3. Pascal, J., H. Stretz, M. Oyanader, P. Arce. "Electrophoresis in Diverging Pores: Role in Modeling Nanocomposite Gels." Revised manuscript available.

## COMPOSITE HYDROGEL MORPHOLOGICAL CONTROL VIA ANISOTROPIC NANOSTRUCTURE INCLUSIONS

Jeff Thompson
Chemical Engineering
Faculty Research Advisors: Dr. Holly Stretz
Collaborator: Dr. Pedro Arce

Nanocomposite hydrogels for have great potential for use in bioseparations of complex protein or DNA mixtures. Previous work has shown that polymers consisting of a native acrylamide matrix embedded with micro/nanostructured thermally responsive polymers, most notably Poly (N-isopropyl acrylamide), have the ability to enhance separation characteristics using gel electrophoresis [1]. By increasing the temperature of the gel beyond the LCST of the PNIPAm/water system, the polymer shrinks creating "macro-voids" in the native hydrogel matrix. In addition to controlling the size of voids, shape control should also have some impact on separation characteristics [2]. Proposed is a route of synthesis of gold nanorods which are surface-modified with a thermally responsive PNIPAm coating. These nanoparticles will then be incorporated into a native hydrogel matrix and the composite hydrogel will be probed using complex protein mixtures that have previously shown low separation efficiencies at temperatures both below and above the polymer LCST. Further work will include modeling efforts to understand the physics of transport of the mixtures.

**References:**
1. Thompson J., H. Stretz, and P Arce U.S. Patent Application 12275253
2. Trinh S., B. R. Locke, and P. Arce, "Diffusive-convective and diffusive-electroconvective transport in non-uniform channels with application to macromolecular separations," Separation and Purification Technology, vol. 15, pp. 255-269, 1999.

## THERMALLY RESPONSIVE MICROPARTICLE GEL ELECTROPHORESIS: NOVEL AND USEFUL METHOD TO IMPROVE BIOSEPARATIONS

Jeff Thompson
Chemical Engineering
Faculty Research Advisor: Dr. Holly Stretz
Collaborator: Dr. Pedro Arce

Nanocomposite gels for drug delivery and bioseparations of proteins or DNA hold great potential. These materials feature, for example, nano or microparticles embedded in the gel structure that creates a thermo-sensitive and composite polymer with different and unique transport properties. The synthesis and characterization of poly(N-isopropyl acrylamide) thermally responsive particles as well as formation of the gel composites are described. The particles are synthesized with a precipitation polymerization crosslinking reaction and subsequently inserted into polyacrylamide gels[1]. In addition, electrophoresis runs are used to test the transport of proteins through the composite. Visual characterization is used to determine and compare the transport (i.e. mobility and dispersion) characteristics of the new gels with standard gels in the electrophoresis runs. Composites are studied with the same polymer and crosslinker concentration of control gels and are studied via the probes Ovum Serum Albumin, Bovine Serum Albumin, and Cytochrome C. Results show separations in a protein mixture which were previously unachievable.

**Reference:**
1. St. John, Ashlee, Victor Breedveld, L. Andrew Lyon "Phase Behavior in Highly Concentrated Assemblies of Microgels with Soft Repulsive Interaction Potentials" Journal of Physical Chemistry. April 30, 2007.

## FATE OF FATTY ACIDS ADSORBED ON EXHAUST DUCT SURFACES DURING COMMERCIAL FAST FOOD COOKING

Kiran K. Thota
Chemical Engineering
Faculty Research Advisor: Dr. Pedro E. Arce
Collaborators: Dr. Dennis B. George and Dr. Martha J.M. Wells (Center for Management, Utilization, and Protection of Water Resources)

Surface science is the study of physical and chemical phenomena that occur at the interface of two phases(i.e. solid-liquid interfaces, solid-gas interfaces and liquid-gas interfaces). When a gas or vapor contacts a solid, some components in the vapor may become adsorbed onto the solid. The molecules removed from the gas either enter the solid, or remain on its surface. Volatile organic compounds and particles( on the order of 10-6 μm) transported in the air exhaust from commercial fast food cooking operations, such as hamburger, chicken fillet, fish fillet and french fries, etc., may adsorb on surfaces of exhaust ducts. The fate of these adsorbed compounds is unknown. Research was conducted to determine the kinetic rates of photo catalytic oxidation of these organic compounds once adsorbed to the exhaust ducts. Furthermore, the research also report on the effect of ozone oxidation in eliminating the organic compounds from the surface. The presentation will describe details as well as preliminary results of the research. Directions for further efforts will be also presented.

## THE SOCCER BALL MODEL: A POWERFUL PoK TO APPROACH UP-SCALING IN THE CLASSROOM

Cynthia Torres and Jennifer Anne Pascal
Chemical Engineering
Faculty Research Advisor: Dr. Pedro Arce

When studying the physics of transport, it is necessary to develop conservation equations for variables such as total mass, energy, and momentum. In order to accomplish this, the concept of a continuum scale must be introduced. Since most students have only been introduced to the physical and chemical concepts related to total mass, energy, and momentum, from a discrete scale point of view, this concept can be very challenging for the student (learner). Most textbooks do not address this issue, assuming that the mathematical steps and concepts are familiar to the learner[1] , when in fact, they are not. This can be frustrating to the student and does not enable them to fully understand or capture the importance of this important idea of a continuum scale. An alternative approach is to design a student-centered activity (Arce and Schreiber, 2004) to engage the student in every step from one scale to the

other. Thus, we propose an approach that uses soccer balls, to help with this transformation process, in conjunction with geometrical domains, mathematical principles, and physical properties. In this contribution, the authors will discuss the soccer ball model from a student's point of view along with its advantages and compare it to more traditional, familiar methods for introducing the concept of a continuum scale. The important role of the SBM as a POK (Arce, 1994; 2000) will be highlighted.

References:
1. Arce, P. and L. Schreiber, "High Performance Learning Environments, Hi-PeLE", Chemical Engineering Education, 286-291, Fall 2004.
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3. Arce, P.; Oyanader, M.; and Whitaker, S. "The Catalytic Pellet: A Rich Learning Environment for Up-Scaling," Chemical Engineering Education, 41(3), 187-194 (2007)
4. Arce, P., "Principal Objects of Knowledge (POK's) in Colloquial Approach Environments," Annual Conference Proceedings, American Society for Engineering Education, ASEE (2000, CD-ROM).

[1]In fact, textbooks suppressed the student opportunity to learn the concept by directly telling the answer. (See Arce et al, 2007).

## DATA MINING PubCHEM WITH SIGNATURE: PREDICTION OF BIOLOGICAL ACTIVITY FOR SMALL MOLECULES

Derick C. Weis
Chemical Engineering
Faculty Research Advisor: Dr. Donald P. Visco

High-throughput screening (HTS) is a technique to discover new lead compounds by physically screening a large library against a specified biological target. HTS was primarily available only to the pharmaceutical industry in the past. Because of the Molecular Libraries Initiative [1], part of the NIH Roadmap for Medical Research, HTS is now accessible to academic researchers where the data collected is deposited in a public database called PubChem. The results from more than 1,000 different HTS experiments are currently readily available in PubChem to download. Cheminformatic tools are crucial to effectively interpret and utilize this vast amount of data. In this work, we demonstrate a method to create a model from existing HTS data in PubChem, and predict new compounds likely to be active for additional screening. PubChem bioassay 846 [2] screened for potential anticoagulant therapeutics by identifying inhibitors of factor XIa, which is involved in the blood coagulation mechanism. A classification model with 89% accuracy was created using a support vector machine (SVM) with the Signature molecular descriptor [3]. Approximately 12 million

compounds deposited in PubChem, but not present in the factor XIa assay, were virtually screened by the SVM. Based on metrics associated with SVM magnitudes and molecular descriptor overlap between candidate molecules with those from bioassay 846, we identified 296 compounds (from the 12 million not previously tested) as active. We are currently working to experimentally verify some of the computational predictions using a 96-well microplate reader.

References:
1. Austin, C.P., Brady, L.S., Insel, T.R. and Collins, F.S. NIH Molecular Libraries Initiative. Science 2004, 306, 1138-1139.
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3. Faulon, J.L., Visco, D.P., Jr. and Pophale, R.S. The signature molecular descriptor. 1. Using extended valence sequences in QSAR and QSPR studies. J. Chem. Inf. Comput. Sci. 2003, 43, 707-720.

## PARTICLE STIMULATE HYDRATION OF PORTLAND CEMENT

Tiantian Xie
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Faculty Research Advisor: Dr. Joseph Biernacki

The chemical reactions that occur during the early stages of portland cement hydration are complicated and the basic mechanisms of hydration kinetics yet debated. In order to get a better understanding of the early stage of cement hydration kinetics and the effect of involved particle properties, tricalcium silicate (the main component in portland cement) was chosen as a model system instead of cement. A new mathematical approach is considered for simulating hydration. Unlike many of the traditional models, nucleation and growth of the products are explicitly included, as well as other mechanistic aspects of the hydration process. Furthermore, molecular diffusion of reactants and reaction rates are distinguished for inner and outer product formation, that product formed by displacement of dissolved reactants at the particle core and that product formed on the surface of growing particles respectively. Various researchers have observed that early stages of hydration are accelerated by the presence of even inert particles. This phenomena can be explained by a nucleation model wherein product growth may occur on otherwise chemically inactive surfaces. Good agreement between the model and experimental data is observed. This strategy is paving the way for more elaborate models based on nucleation, growth and population balance methodologies.

# CHEMICAL ENGINEERING
## UNDERGRADUATE STUDENTS

### PRE-PROCESSING BIOMASS FOR FAST PYROLYSIS EXPERIMENTS

Martin Bijou
Chemical Engineering
Faculty Research Advisor: Dr. Joseph Biernacki

In today's volatile energy market, interest in biomass and biofuels is at an all-time high. As the world's supply of fossil fuels is depleted and green house gasses continue to be pumped into the atmosphere, the scientific community has both a moral and pragmatic obligation to seek new energy forms with minimal or no impact on the environment. We are considering plant cellulose as a possible solution, though many obstacles remain. One route is fast pyrolysis, however, the kinetics of reaction are yet not fully understood. Our TTU team is actively developing a tiny fast pyrolysis reactor that may help to elucidate kinetic behavior. Introducing the biomass into the hot reactor, however, remains a significant challenge. One approach requires a tinny spherical bead of material no more than 500 microns in diameter. The goal of this research is to find a way to take raw cellulosic biomass and manipulate it into the form of spherical particles that are small enough for use in the TTU fast pyrolysis reactor.

### FIBER FILM REACTOR: EFFECT OF FLOW ON A TWO PHASE SYNTHESIS OF GOLD NANOPARTICLES

Martin Bijou
Chemical Engineering
Faculty Research Advisor: Dr. Holly Stretz

The nature of fiber film reactor performance is being evaluated. Preliminary data revealed that some back mixing is occurring at *** ml/min in a bench-scale prototype reactor. Evidence of this was that the residence time distribution for gold nanoparticles (the solute, about 5nm in diameter) in a pulse injection experiment was broad. The gold nanoparticles, however, could be adhering to the fiber surface and this might cause the observed band spreading, rather than fluid turbulence. Therefore, pulse injection of a solute which is molecular in size, methylene blue, is planned to help understand the role of fluid dynamics in the capillary pores of the reactor. The overall project goal is to find operation windows for which a two phase "falling film" can be effectively used to grow gold nanoparticles in a restricted nano-scale phase and potentially produce a narrow distribution of gold nanoparticle sizes.

### THE INTERGRATE METHOD: A NOVEL APPROACH TO PHASE EQUILIBRIUM CALCULATIONS

Drew Blumberg and Seth Wynne
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Faculty Research Advisor: Dr. Donald P. Visco, Jr.

Calculation of system phase properties for chemical species in equilibrium generally requires the equality of phase pressures and temperatures, as well as equality of either chemical potentials or fugacities of each component across all system phases. Once these equations have been written, the solution of the problem generally relies upon the numerical techniques of applied mathematics. Unfortunately, the traditional numerical methods for solution are often slow and require many steps to create the entire coexistence curve, especially for mixtures. In this work, we explore two methods for the resolution of these difficulties. Rather than using a root-finding approach, one can utilize a differential approach wherein one integrates differential equations to trace the coexistence curve. This novel technique, known as the integrate method, does not have the same pitfalls as the root-finding approach, though it does have other limitations. An alternative to this is to explore the possibility of a purely analytical implementation of the integrate method to solve phase equilibrium problems.

### SUPERCOOLED WATER MOVEMENT WITHIN A PEM FUEL CELL

David J. Dearmon
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Faculty Research Advisor: Dr. Cynthia Rice-York

Proton exchange membrane fuel cells are a potential solution to alleviate dependence on foreign oil by replacing the internal combustion engines in automobiles. Water is intrinsic to PEMFC's, both for adequate hydration and as a reaction byproduct. For automotive applications, hundreds of individual fuel cell repeat units are stacked together in a series to create a higher output. Massive endplates are used to compress the stack and they act as thermal sinks during freeze. At subzero temperatures the water within the catalyst layers of the PEMFC remains unfrozen in a supercooled state, to temperatures as low as -48°C. The supercooled water moves due to temperature gradients induced by the endplates during freeze through capillary forces towards the freezing boundary. Supercooled water moves and collects forming ice lenses increasing the resistance of the cell and restricting reactant flow. A restriction to flow lowers the output efficiency of the cell. The rate at which the supercooled water moves from the catalyst layers can be quantified by monitoring resistance, temperature, and

pressure gradients within the PEMFC. The goal of this project is to understand supercooled water mobility as functions of material and environmental properties and to specify criteria for freeze tolerant PEMFCs.

## ANALYSIS OF DIALYZER PERFORMANCE IN AIDING KIDNEY FUNCTION

Katie Frederick
Chemical Engineering
Faculty Research Advisor: Dr. Pedro E. Arce

One of the key systems in the human body assisting in cleaning blood is the renal system with a unique anatomy and physiology to perform the various and complex functions. Many components are included in this system including arteries, veins, and its central organ, i.e. the kidney. This is, in fact, in "composite" domain where "smaller" scales components are located in an efficient and relatively compact space. The kidney contains many components that make up the whole system. The two main areas of the kidney are the cortex and the medulla. The cortex contains 85% of the kidney's main unit of function, the nephron. It also contains capillaries, which direct the flow of blood through the cortex. The medulla contains the renal pyramids and most of the arteries and arterioles. Part of the nephron, the Loop of Henle, dips deep into the medulla. All of these components are neatly fitted together to perform specific functions. Aiding devices to assist patients with a non-regular performing kidney include the so-called dializers that have been designed to mimic (at to a point) the complex functions of the kidney. For example, the kidney balances the composition of blood and water, and it filtrates urine. Determining what causes these functions to fail is the key to improving dializer performance. In this research proposal, we are interested in formulating a suitable mathematical model based on differential equations and boundary conditions to study the "filtration functions" of the dializer performance. Several aspects related to this proposal will be discussed in the proposed poster.

## BENCH SCALE STUDIES OF THE THERMAL CONVERSION OF BIOMASS THROUGH FAST PYROLYSIS

Tiffany Hughes
Chemical Engineering
Faculty Research Advisor: Dr. Joseph Biernacki

Pyrolysis is a thermo-chemical process that converts organic materials into usable fuels by heating biomass until it separates into a solid and gaseous state. The gas can then be condensed to form bio oil from the biomass constituents. Pyrolysis is a fast, direct method of biomass conversion into energy fuel and could prove to be highly competitive in industry as non-renewable fossil fuel resources are replaced.

Many uncertainties still exist in the chemical pathways that lead to the production of the bio oil since this technique is still in early development. The large number of experimental variables contributes to the complexity of the problem. The choice of feed materials, heating rates, sample sizes, and carrier gases may cause variations in the resulting products. Two methods of pyrolysis are being viewed in this study. A fast pyrolysis fluidized bed reactor is being constructed that will utilize the efficient transfer of heat from a sand bed to convert biomass into a gaseous state. The vapor will then be condensed into bio oil. This method is being used in research on a large scale and provides a highly visual way to monitor the biomass conversion process. The second method used is thermogravimetric analysis (TGA) which monitors the thermal degradation of biomass over a specified heating range. This provides information about the temperatures at which the biomass dries and pyrolyzes. Gas chromatography can then be used to study the bulk composition of the gaseous effluents. The biomass feedstock for both experiments includes a variety of grass strains obtained from a TTU affiliated farm. Fescue straw and orchard grass are being used in current studies.

## DISPERSION OF NOVEL CARBON NANOTUBES IN POLYETHYLENE: HOT COAGULATION METHOD

Azuráe K. Johnson
Chemical Engineering
Faculty Research Advisors: Dr. Holly Stretz and Dr. Pedro Arce
Collaborator: Dr. Vijay John (Tulane University)

The hot coagulation method is a way to premix nanoparticles in high polymers prior to compounding/molding of test bars1. The objective is to maximize dispersion of (in this case) carbon nanotubes (CNT) in maleic-anhydride modified polyethylene. The test bars were tested for Young's modulus, rheology, electron microscopy, visual clarity and percent crystallinity. The novel carbon nanotubes used are a patented material in development at Tulane University (Dr. Vijay John's group.) This type of characterization will allow us to use composite theory to back-calculate the properties of the synthesized CNT. Good dispersion is an important assumption in these calculations, thus the experimental work requires rigorous attention to this important parameter.

## REPRODUCIBILITY OF OSA MOBILITY IN TEMPLATED GELS UTILIZING GEL ELECTROPHORESIS

Azuráe Kayla Johnson and Jeffery Thompson
Chemical Engineering
Faculty Research Advisors: Dr. Holly Stretz and Dr. Pedro Arce

OSA, or ovum serum albumin, is used in this study as a model for a drug or biological marker (in blood serum this could be the LDL or HDL markers for instance). Our overall goal is to provide researchers with novel ways of separating complex mixtures of drugs (proteins). Efficient separation would enable pathways to drug purity and enable diagnostic techniques with better definition of the results. The templated gel in this case is a novel material that changes morphology on the nanoscale with a bulk change in temperature, so that the separation can be "tuned" by the researcher. Reproducibility is a key issue, and here we have characterized that as +20% for bandwidth and + 1% for movement of the protein along the lane. Future work will allow us to compare these experimental results with computational predictions of optimal time to resolution in electrophoretic flows through nanochannels.

## IONIC LIQUIDS: A PRETREATMENT FOR CELLULOSIC ETHANOL

Alex Meyers
Chemical Engineering
Faculty Research Advisor: Dr. Donald Visco

Although the true potential of ionic liquids has yet to be ultimately discovered, in recent years much research has been dedicated to finding new areas of their application. Ionic liquids are commonly referred to as "green solvents" due to their lack of vapor pressure, which makes them easily recoverable. Our research revolves around the possibility of using ionic liquids during the pretreatment stage of the production of cellulosic ethanol. This pretreatment process is traditionally performed using acid hydrolysis or high temperature/pressure conditions and is meant to expose the cellulose from the tightly bound lignin. We are investigating using ionic liquids in order to dissolve cellulose, which would isolate it from the lignin. Only a handful of ionic liquids have been found to dissolve cellulose up to 15% by mass. (Zhao,2008) Other ionic liquid properties we are exploring include low melting point and low viscosity, which minimize energy inputs. In this work, we have used our inverse-design approach with signature to identify novel ionic liquids with predicted properties, optimized for cellulose pretreatment and further evaluation. (Churchwell, 2002) In addition, we have constructed an apparatus to experimentally test the solubility of cellulose in ionic liquids.

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## SOLUBILITY OF BLOWING AGENT IN POLYOLS

Andrew Parkes
Chemical Engineering
Faculty Research Advisor: Dr. Donald P. Visco, Jr.

The overall goal of this research is to develop useful polyol/blowing agent pairs which are integral to producing polyurethane foam. Previous blowing agents used were discovered to be harmful to the environment and hydrofluorocarbons have been identified as potential long term replacements. These blowing agents do not contain any chlorine and, therefore, are not ozone depleting. The solubility of the blowing agent in a particular polyol determines the quality of the polyurethane foam that is created. Therefore, our objective is to determine the solubility of HFC's in a variety of polyols. Thus far, experimentation has included some of the most common HFC's used in industry today such as pentafluoroethane (HFC-125), difluoroethane (HFC-152a), trifluoroethane (HFC-143a), and difluoroethane (HFC-32). The polyols that were utilized include Pluracol ® 975 a Polyether-based sucrose polyol with high functionality (-OH groups), Pluracol ® 355 an amine-based tetrol also with high functionality, and finally Terol ® 352 an aromatic polyester polyol with low functionality. Currently, research indicates that good solubility is realized when bonding between the polyol and the blowing agent is favorable for hydrogen bonding. Future work will potentially further validate this finding and utilize a thermodynamic model to predict optimal blowing agent/polyol systems.

## CHARACTERISITICS OF A FIBER – FILM REACTOR FOR TWO PHASE OPERATION

Zach Seibers
Chemical Engineering
Faculty Research Advisor: Dr. Holly Stretz

The two-phase reactor is designed to maximize the surface area available for reaction. This prototype reactor could one day produce a fluid dynamics simulation of flow and prevent solutions from separating after their reaction. The primary goal of this research is to develop a usable model for the

reactor so that accurate predictions can be made about the reactions that it will host in the future. The research done to date has been to design a general model for the reactor and now we plan to improve the model to be more specific to our reactor. Gathering information on the geometry of the fibers in the reactor, calculating the Residence Time Distribution, and determining the flow profile of the fluid are steps taken to generate an accurate usable model for the reactor.

## ZETA POTENTIAL MEASUREMENTS OF GOLD NANOPARTICLE IN HYDROGELS

Melissa Taylor and Vasanta Pallem
Chemical Engineering
Faculty Research Advisors: Dr. Pedro Arce and Dr. Holly Stretz

Zeta potential is the electrostatic potential of the nanoparticle within the interfacial double layer at the slip plane. In this research project, the potential difference between the dispersion medium and the stationary layer of fluid attached to the dispersed nanoparticle was studied, measured, and evaluated by the Environmental Protection Agency and was then gold nanoparticle movement and aggregation in hydrogels was reviewed. Model equations represent the relationship of zeta potential versus the charge in nanoparticles have been developed from Smoluchowski. Furthermore, experimental techniques suitable for the measurement of zeta potentials have been used to evaluate zeta potential-particle gradient relationships. By implementing experiments using both equations and zeta-phorometers provided by the EPA, zeta potentials were used to make predictions of surface charged of the nanoparticles and their variances in different gel compositions.

## USING THERMOPOROSIMETRY TO CLASSIFY PORE SIZE DISTRIBUTIONS IN NAFION®-115 MEMBRANES

Jonathan Wheeler
Chemical Engineering
Faculty Research Advisors: Dr. Holly Stretz, Dr. Pedro Arce, Dr. Joseph Biernacki, and Dr. Cynthia Rice-York

Using a differential scanning calorimeter (DSC), our group will examine these NAFION®-115 membranes using a method known as thermoporosimetry. This technique will help us to determine and classify the pore size distribution of these membranes. The goal of these experiments is to observe any changes in pore sizes of these membranes with the relative humidity in which they were conditioned. A brief description of the physics behind thermoporosimetry and the purpose of these membranes will be provided.

## DESIGN OF INHIBITORS FOR AMYLOID BETA PROTEIN OLIGOMER AGGREGATION THROUGH I-QSAR AND SIGNATURE

Joshua S. Williams
Chemical Engineering
Faculty Research Advisor: Dr. Donald P. Visco Jr.

We present in this research a means to prevent the detrimental effects of Alzheimer's disease by targeting the aggregation of amyloid beta protein oligomers through small molecule inhibition. Alzheimer's disease is the most common form of dementia, afflicting over 26 million worldwide, and the number of individuals who develop Alzheimer's is expected to grow rapidly in the future. The symptoms of Alzheimer's include confusion, language breakdown, and eventual loss of memory and vital bodily functions, as well as the notable development of amyloid beta plaques in the brain. As the monomers of amyloid beta begin to aggregate, they form a soluble, toxic intermediary which has been linked to neuronal cell damage. Therefore, our solution is to use small molecule inhibition to form a barrier preventing the formation of soluble aggregates. In order to develop the most effective compounds to accomplish this, will we be using the inverse-quantitative structure-activity relationship algorithm with the Signature molecular descriptor. Our goal is to generate compounds through advanced computer-aided molecular design which fit a desired, predicted profile. The synthesis and confirmation of these compounds will be performed by colleagues at the University of South Carolina.

# CIVIL AND ENVIRONMENTAL ENGINEERING
## GRADUATE STUDENTS

## APPLICATION OF NON-TRADITIONAL U-TURN BASED TREATMENTS AT NARROW-BRIDGED DIAMOND INTERCHANGES

Chris Berry
Civil and Environmental Engineering
Faculty Research Advisor: Dr. Steven Click

The objective of this thesis was to analyze the application of non-traditional U-turn based interchange treatments at narrow-bridged interstate interchanges. I-75 at APD 40, I-40 at Genesis Road, and I-40/75 at Watt Road served as the tests sites for the research. A simulation model of each non-traditional treatment was created for each of the three sites using VISSIM, a microscopic traffic simulation model. The simulation models emulated real-life performance while recording vehicle travel times and ramp queue lengths. All of the non-traditional treatments significantly

improved the interchange performance characteristics. The non-traditional treatments investigated were the Median U-turn Interchange, Superstreet Based Interchange, and the 'Free Range Eagle' Interchange. The more traditional Single Point Urban Interchange (SPUI) was also investigated for comparison. None of the investigated treatments except the SPUI modified the interchange bridge. The 'Free Range Eagle' Interchange undoubtedly out-performed all of the non-bridge modifying treatments studied in both this thesis as well as treatments previously analyzed. The SPUI, which widens the interchange bridge, provided superior performance across the test sites. However, the results of the non-bridge modifying treatments indicate that they could be used to significantly improve congestion and performance of narrow-bridged interchanges without modifying the existing bridge structure.

## FACTORS AFFECTING UNDERGRADUATE ENROLLMENT IN ENGINEERING FROM RURAL COUNTIES

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This study presents a comprehensive statistical analysis of engineering enrollment at the undergraduate level in TTU to identify factors of low enrollment from rural counties. While there exists a considerable difference in enrollment between urban and rural counties that can be explained by factors such as income level and average education level of the population, this study clearly verified that there is statistically no significant difference between the capabilities of rural and urban high school students in terms of ACT and SAT scores. It was diagnosed therefore that more outreach activity, utilizing the publicity of exciting engineering research that is carried at TTU could potentially raise awareness among rural high school students of the careers in engineering.

## RISK ANALYSIS OF DAM INFRASTRUCTURE IN TENNESSEE

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This study presents a risk analysis study for the oldest dam in the Tennessee River basin – the Wilson dam. The historical flow at the dam site was fitted to Generalized Extreme Value (GEV) distribution using the L-Moment method. The theoretical flow estimated by the distribution matched very well with the historical (observed) flow. From the analysis, hydrologic risk was computed for various hypothetical return period scenarios. If the dam was designed for a flood

with a return period of 10,000 years, the dam was found generally safe. In contrast, high values of hydrologic risks were obtained for the 1000 year return period flows. Analysis using the L-moment method showed that the Wilson dam is potentially under high risk if it was designed for a flood magnitude having a return period of 1000 years or less. Because most dams around the world are designed for a 500 year return period, this study underscores the need for a reevaluation of risk for ageing dams. Furthermore, this technical note also demonstrates the unique value of the L-moment method in incorporating post-dam flow data for a more robust risk analysis.

## UNDERSTANDING THE INFLUENCE OF LARGE DAMS ON ALTERING EXTREME PRECIPITATION VARIABILITY

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Very little is known on the vulnerability of dams and reservoirs to man-made alteration of the extreme precipitation and flood as we step into the 21st century. This is because conventional dam and reservoir design over the last century has been 'one-way' with no acknowledgement of the possible feedback mechanisms affecting the regional water cycle. Although the notion that an impoundment could be built to increase rainfall was suggested more than 60 year ago dam design protocol in civil engineering continues to assume as 'static' the statistical parameters of a low exceedance probability precipitation event during the lifespan of the dam. This study, using a global dam and precipitation database spanning more than 6 decades has shown that the extreme precipitation has indeed been altered considerably under certain circumstances. It is time for us to change our perceptions and embrace a hydrometeorological approach to dam design and operations.

## PROTON NMR: A NOVEL APPROACH FOR CHARACTERIZING THE DURABILITY OF HIGH PERFORMANC CONCRETE

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The ability of concrete to resist cracking, weathering action, chemical attack, and abrasion while maintaining its desired engineering properties is linked to the observation and monitoring of water movement in concrete. Unfortunately, the lack of capable systems for monitoring moisture movement in concrete has remained a challenge. In order

to improve the present state of knowledge concerning the water transport kinetics in concrete, 1H nuclear magnetic resonance (NMR), an in situ nanoscale characterization technique, has been identified as a revealing tool for assessing changes in water mobility in porous cementitious matrices at early ages. This study investigated the application of NMR spectroscopy at monitoring changes in the early age hydration of cement as well as the effects of internal curing; an important mitigation strategy to resist shrinkage and cracking in high performance concrete.

## INVESTIGATING THE TRANSFER OF SATELLITE RAINFALL INFORMATION FROM GAUGED TO UNGAUGED LOCATIONS

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A fundamental paradox of satellite rainfall data is that it is most useful over ungauged locations where there is no way of deriving uncertainty information directly using ground validation (GV) data. This study investigates how much error information can be 'transferred' from known locations to ungauged points using a geostatistical spatial interpolator. The method of ordinary kriging was implemented on mid-western United States assuming that 50% of the region lacked GV rainfall data. Various error metrics were interpolated for the non-GV grid boxes (for which the true error metric value was known a priori) using kriging and a nearest neighborhood window (of size equivalent to the correlation length of the metric). This process was repeated for 10 realizations of randomly selected gridboxes (comprising 50% of the total domain) and the accuracy of kriging was then assessed statistically. Preliminary results indicate that kriging has promise for transferring error information to ungauged locations, particularly for Probability of Detection (POD) and RMSE. Table 6 below shows the summary of accuracy of kriging for various error metrics. Future extension of this work will test the role played by % missing

## HIGH PERFORMANCE LIGHTWEIGHT CONCRETE

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There has been a substantial amount of research performed pertaining to lightweight concrete, and also to high performance concrete (HPC). There has been very little research performed involving high performance lightweight concrete. This research project is geared towards developing a high performance lightweight concrete mixture that is both practical and economical enough for field use. HPCs are advantageous because of improved strength and durability properties. HPCs exhibit higher compressive strengths and a lower permeability than ordinary concrete mixtures. The use of HPCs also tends to decrease total job cost. The use of lightweight concrete is advantageous because of improved thermal and sound insulating properties, along with a decrease in the design dead load of a structure. It seems then, that a concrete mixture that contains all these qualities would be very beneficial to the construction industry, given the industry takes the initiative and begins to use an unprecedented concrete mixture.

# CIVIL AND ENVIRONMENTAL ENGINEERING
## UNDERGRADUATE STUDENTS

### THE NASA GLOBAL FLOOD DETECTION SYSTEM AND ITS VALIDATION

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Currently, NASA has developed a satellite-based flood detection system using as the primary input, the Tropical Rainfall Measuring Mission (TRMM) Multi-satellite Precipitation product 3B42RT available globally in real-time. This system is expected to evolve to the planned Global Precipitation Measurement (GPM) mission due for launch in 2013. One goal of this NASA Global Flood Detection System is to provide pseudo real-time river discharge or surface runoff information that developing nations, among other users, could use to monitor the evolution of possible flooding. The current challenge now is to determine if the globally modeled runoff data, like that available through NASA's flood detection system, is comparable enough to conventional and in-situ (measured) data at the scale of estimation. The objective of this study is to first understand the NASA Global Flood Detection System. The next objective is to perform a statistical variability of in-situ (hereafter called GV) stream flow data of Bangladesh rivers in relation to NASA satellite rainfall products for eventual validation. Cross correlation studies are performed between NASA rainfall data and observed streamflow data. Preliminary results indicate that NASA real-time rainfall products have considerable hydrologic information for flood forecasting.

## CONCRETE EXPANSION DUE TO DELAYED ETTRINGITE FORMATION

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This research is aimed at investigating the mechanisms of delayed ettringite formation (DEF) causing expansion in portland cement mortars. DEF typically occurs in heat cured, precast, and mass concrete and is increasingly observed in concretes that have been in service for many years. In this research, physical expansion testing was used to measure length changes and environmental scanning electron microscopy (ESEM) was used to evaluated chemical changes. It is well known that ettringite formation is an expansive reaction that may cause cracking. However, little is known about the mechanisms of late age ettringite formation, specifically how different processes can ultimately lead to the same result. The objectives of this research are: (1) to identify those cement composition and mix design factors that lead to macro-scale expansion; and (2) to evaluate the micro-scale chemical changes that occur in the microstructure during heat curing and subsequent storage. Research is ongoing to elucidate and couple the physical testing results with ESEM observations.

# ELECTRICAL AND COMPUTER ENGINEERING
## GRADUATE STUDENTS

## OPTIMAL REACTIVE POWER GENERATION SCHEDULE

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The reactive power generation schedule in a power system determines the bus voltage profile. The available reactive power capabilities of the generators have to be optimally deployed so that bus voltages are kept within specified limits. The basic feature of the new approach in this research tends to recognize the weak coupling between real power flow and voltage. This facilitates focusing on the voltage/reactive power problem keeping the real power flows fixed to values determined from a base case load flow analysis. The reactive power flow in each line will determine the voltage drop in each line and indirectly the bus voltage profile. The line reactive power flows and the bus reactive power injections are kept in focus by writing two sets of equations, viz., reactive power balance at every bus including the slack, and line voltage drop equations. Generator reactive power injections are kept as variables and the total set of equations constitute the equality constraints. The objective function is to minimize the total generated reactive power. Reactive power generation limits and/or bus voltage magnitude limits are specified as allowable range of values of these variables in an optimization procedure using Genetic Algorithm (GA).

## A NOVEL SCALABLE ADAPTIVE SYNCHRONOUS CONTROLLER FOR SIMULTANEOUS MULTI-CHANNEL DATA ACQUISITION SYSTEM

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Existing multi-channel data acquisition systems (DAQ) of heterogeneous input signals either use a super fast analog to digital converter (ADC) with homogenous sampling rate, or dedicated ADC for each channel. Both of these solutions are in-efficient, and/or expensive. In addition, they become infeasible for the acquisition of large number of simultaneous channels (> 16 channels). In this research, a novel heterogeneous simultaneous multi-channel (DAQ) is proposed, with a novel scalable adaptive controller. It is designed to detect the input signal frequency range in order to determine the appropriate sampling rate for each input signal. This provides flexibility to the required sampling frequencies, reduces circuit size and power consumption, and improves the scalability of the multi-channel DAQ systems. An analog multiplexer is adaptively controlled to optimally switch between the acquired analog signals. The acquired data is stored into Flash memory for further analysis and/or archiving purposes. The ADC interface, the storage driver and the adaptive controller are implemented in the FPGA. The proposed system can be used in various applications that require high-quality, reduced cost, low power consumption and small circuit size for the heterogeneous multi-channel data acquisition. The concepts presented are feasible for arbitrary large number of simultaneous channels (i.e., >16). A system prototype was successfully implemented and tested using FPGA. The worst-case prorogation delay observed for the system is 12.04 ns. The Cyclone-II FPGA consumes power as low as 12 mW. Finally, the obtained signal to noise ratio reaches 73 dB per channel.

## NOVEL POWER SYSTEM STABILIZER (PSS) USING WIDE AREA FREQUENCY INFORMATION FROM FNET

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In the 1950s and into the 1960s, many power generating plants were equipped with continuously acting Automatic Voltage Regulators (AVRs). As the number of power plants with AVR grew, it became apparent that high performance of these voltage regulators also had a destabilizing effect on the power system. Power oscillations of small magnitude and low frequency often persisted for long periods of time. In some cases, this presented a limitation on the amount of transmittable power within the system. Power System Stabilizers (PSSs) were developed to aid in damping of these power oscillations. The PSS is an additional control that is part of the excitation system for generator voltage control. The PSS acts to modulate generator field voltage to damp electrical power and/or frequency oscillations. This research is an investigation into modifying one of the inputs of the PSS; namely the frequency. Instead of using the frequency of generator on which the PSS is installed (which is the traditional practice), the use of wide area frequency measurements is suggested in this study. The wide area frequency measurements are available from the Frequency monitoring Network (FNET) system. The FNET system is a new concept and is being developed and presently installed.

## NEURAL NETWORK APPROACH TO THE PREDICTION OF PERCENTAGE DATA PACKET LOSS FOR WIRELESS SENSOR NETWORKS

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Wireless sensor networks are used in the field of communications and have gained enormous popularity in recent times. Depending upon the environment in which the wireless sensor network operates, the amount of noise level would differ and hence the data packet loss in wireless communication would vary. This paper presents a solution to the prediction of percentage data packet loss in the wireless sensor network in indoor and outdoor environment. It uses the Artificial Neural Network (ANN) to predict the data packet loss and the Erasure Coding technique to find the actual percentage data packet lost in wireless sensor network. The results obtained from the ANN are compared to the respective ones yielded by the Erasure Coding technique and are found to exhibit satisfactory accuracy.

## AN AVAIABILITY BENCHMARKING SIMULATOR FOR DISTRIBUTED FILE SYSTEMS

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Motivated by the requirement of large-scale data processing in both scientific and business applications, modern distributed file systems not only need high performance, but also must ensure the availability of its functionalities. However, with the increase of both the number of computer nodes and the population of clients, the challenge of designing a highly available distributed file system becomes more critical than before, given that failures are a commonplace characteristic in such systems rather than an exception [1, 2, 3]. In this paper, we propose an availability benchmark simulator which aims to to provide a comprehensive evaluation of availability for distributed file systems under various faulty scenarios. There are three major benefits of the simulator: 1. it enables reasoning about existing file system mechanisms; 2. it simplifies the introduction and adoption of new fault tolerance techniques in a distributed file system; 3. it helps to locate the potential bottlenecks and major overhead contributors in a distributed file system.

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## MODELLING, ANALYSIS AND OPERATION OF MICROGRIDS

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Microgrids have gained research interest during the last few years largely due to exponential global demands on clean energies, especially the drive to mitigate greenhouse gas emissions. Today, it is believed to be the future of power system, providing economic and environmental benefits. To ensure reliable microgrid system, a well-designed model for its operation is expedient. An adaptive controller is required to coordinate the different Distributed Generation (DG) resources based on the load-generation balance in the microgrid, and status of the ac grid. However, despite the strengths of microgrids, it is besieged with numerous technical operational constraints such as DG interface problems and protection issues. This research aims to develop an efficient microgrid structure that addresses these problems without compromising quality of electricity

supply to consumers. The DGs for the Microgrid system in this research shall be: Photovoltaic cells, Fuel cells, Wind and micro-turbines. Behavior of the model when operating in stand-alone mode and grid-connected mode shall be investigated. The credibility and overall performance of the developed system shall be evaluated using RTDS simulations and compared with results of other researchers.

## A WIDE FREQUENCY BAND CIRCUIT FOR MEASURING MUTUAL CAPACITANCE WITH APPLICATION TO MONITORING OF METAL FILL PROFILE

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Collaborator: Dr. P. K. RAJAN

A novel low cost, high frequency circuit for measuring capacitance is proposed in this work. This new capacitance measuring circuit is able to measure small coupling capacitance variations with high stray-immunity. Hence, it could be used in many potential applications such as measuring the metal fill time in the Lost Foam Casting (LFC) process and Electrical Capacitive Tomography (ECT) system. The proposed circuit is based on differential charging/discharging method using current feedback amplifier and a synchronous demodulation stage. The circuit has a wide high frequency operating range with zero phase shift; hence multiple circuits can work at different frequencies simultaneously to measure the capacitance. The non-ideal characteristic of the circuit has been analyzed and the results verified through LTSpice simulation. Results from the tests on a prototype and a simulation elucidate the practicality of the proposed circuit

## KVM ON CLUSTERS: TACKLING THE DISK I/O BOTTLENECK FOR HPC VIRTUALIZATION

Ben Eckart
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I/O efficiency in virtualized environments, specifically with respect to disk I/O, remains little understood and hardly tested. Our research goal is to analyze the properties of disk I/O in virtualized cluster environments in order to identify, study, and eventually minimize all possible performance bottlenecks. As part of our ongoing research, we have developed an extensible performance analysis framework for characterizing disk I/O workloads across virtualized clusters. This poster focuses on the disk I/O characteristics of the Kernel Virtual Machine (KVM). Using our framework within KVM, we are able to conduct extensive tests to determine an accurate characterization of disk

I/O in relation to these factors: multicore, disk scheduling, paravirtualization vs. full-virtualization techniques, caching effects, and networked storage configurations. Our poster reflects our ongoing virtual I/O research, displaying the uses of this novel framework for the HPC virtualization community, and discusses preliminary analysis of our results on a small-scale cluster configuration.

## A NEW FEATURE BASED SOLUTION TO FORWARD PROBLEM IN ECT

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A new feature based technique is introduced to solve the Forward Problem (FP) in Electrical Capacitance Tomography with a target application of monitoring the metal-fill profile in Lost Foam Casting (LFC) process. The new technique for solving FP is based on extracting key features from given metal distributions and then training a Neutral Network with these features. The output of Neutral Network is a scaling factor that modifies the linear sensitivity matrix traditionally used in the solution of the FP. The training and testing data is generated through ANSYS and MATLAB simulations. This approach shows promising results. The Neural Network was able to learn the effect of these features on scaling factor. The RMS error for training distribution was 1.94% and for test distribution, it was in between 2% to 15% depending on the electrode pair with an average of 5%.

## DYNAMIC FREQUENCY ESTIMATION OF BUS VOLTAGES

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New monitoring devices such as Phasor Measurement Units (PMUs) and Frequency Data Recorders (FDRs) have been added to power systems recently. PMUs are placed at various substations to measure voltage and current phasors as well as the frequency of the system voltage. FDRs (relatively inexpensive compared with PMUs) are connected at low voltage (110 V) and measure the system frequency at different locations. It is anticipated, these frequency measurements will be used for real time control of power systems in near future. This research is focused on developing a dynamic frequency estimation technique that simulates the PMU and/or FDR measurements. The technique uses the fact that the voltage at any point of the power system is the sum of voltages contributed by all generators and thus is a multi-frequency voltage involving the frequencies of all generators. Assuming a single-frequency voltage, the frequency is calculated such that the difference between this voltage and the actual voltage is

minimized. The developed frequency estimation technique is coded so that it can be used in conjunction with existing simulation packages. The estimation technique is performed on various IEEE test systems.

## BATTERY CHARGING POWER ELECTRONIC CONVERTER AND CONTROL FOR PLUG-IN HYBRID ELECTRIC VEHICLE

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A plug-in hybrid electric vehicle (PHEV) is defined as any hybrid electric vehicle which contains: A battery storage system of 4 Kwh or more used to power the motion of the vehicle, a means of recharging that battery system from an external source of electricity; and an ability to drive at least ten miles in all-electric mode and consume no gasoline. The conversion from hybrid electric vehicle to plug-in hybrid electric vehicle is achieved by adding a high energy density battery pack in order to extend the all-electric-range (AER). The battery pack of PHEV must be able to store energy from external charging as well as from regenerative braking and must be able to supply stored energy back to the utility as well. Hence, an AC outlet charging system would need a battery charger for the PHEV. Uncontrolled rectifiers and line commutated phase controlled rectifiers so far dominated the AC to DC power conversion. Such converters have inherent drawbacks such as harmonics in the input current and output voltage; low input power factor especially at low output voltage. These classical power converters draw non-sinusoidal input ac currents leading to low input power factor and injection of harmonics into the utility line. The PHEV battery charger requires a Power Factor Correction (PFC) based AC-DC converter which comply with the standards like IEC 61000-3-2 and IEEE 519-1992. These converters have high efficiency, inherent power quality improvement at the ac input and dc output. Another aspect that needs to be considered is the inclusion of a Bi-directional DC-DC converter, that is both taking power (during charging) and providing power (during discharging) from/to the grid (and the vehicle). The charging current from regular power outlet could reach hundreds of amperes depending on charging time. Typical charging time could take hours. Thus, a fast charging is a desirable option, a novel effective charging control has been discussed and analyzed.

## SURFACE POTENTIAL BASED ANALYTICAL MODEL OF HIGHLY ASYMMETRICAL INDEPENDENT DOUBLE GATE DEVICES

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The ever increasing need for enhancement in CMOS performance has given rise to accelerated research in Non-classical multi-gate transistors. Classical form of research focused on bulk devices and used threshold based models to analyze their characteristics. Recent research work has introduced a novel approach to analyzing and modeling symmetrical devices using surface potential approach as opposed to age long threshold voltage based approach. This poster aims at modeling highly asymmetrical independent devices using the new surface potential approach. The effects of various parameters like silicon thickness, oxide thickness, and work functions of top and bottom gates are studied and analyzed extensively as a part of this work.

## IMPROVEMENT OF AREA CONTROL ERROR (ACE) USING FNET DATA

Anish Joshi
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Area Control Error (ACE) is used as the input for the Automatic Load Frequency Control (ALFC) loop in interconnected power systems. Calculation of ACE involves the net area power exchange and the area frequency deviation. An accurate ACE is essential for the effective operation of the ALFC loop. This research is an investigation into modifying the frequency component of the ACE. Instead of using the frequency of major generators in the area (which is the present practice), the use of wide area frequency measurements is suggested in this study. The wide area frequency measurements are available from the Frequency monitoring NETwork (FNET) system. The FNET system is a new concept and is being developed and presently installed within the power systems. The application of the modified ACE in ALFC loop is evaluated through simulation of various IEEE test systems using PSS/E software package.

## TRANSMISSION LOSS ALLOCATION IN RESTRUCTURED ELECTRICITY MARKET

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In this research, a new method for allocating transmission losses to restructured market participants is proposed. The proposed method is fundamentally based on Bialek's "Tracing the flow of electricity" method. According to Bialek's tracing method, the generation contribution of all generators in supplying a specific load, or the share of the output of a specific generator used to supply all load demands are determined. In order to allocate losses to loads, the value of each generator-load pair transacted power of the network must be obtained from Bialek's tracing method.

Using calculated transacted power and Z-bus matrix of the network, the loss of this transaction can be calculated as fraction of the total losses caused by the generator. This loss is considered as loss weight factor (LWF). The sum of the LWF values of the specific load related to all generators is defined as Demand Loss Weight Factor (DLWF) of that load. Same approach is used in order to calculate loss weight factors for generators; The sum of the LWF values of the specific generator related to all loads is defined as Generator Loss Weight Factor (GLWF) of that generator. For all loads and generators of the network, DLWFs and GLWFs are calculated and are normalized, respectively. These factors are used to allocate losses to participants.

## A SAG MONITORING DEVICE BASED ON A CLUSTER OF CODE BASED GPS RECEIVERS

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A relatively new technique of differential global positioning system (DGPS) has potential to measure sag on an overhead transmission line conductor. The technique relies on the information received from GPS satellites and carrier based receivers so that sag can be measured to an accuracy of approximately 1" [1, 2]. However, the overall cost of the carrier based system is extremely high. An alternative method based on using a cluster of cheap GPS receivers was explored for the first time and proposed. A single code based GPS receiver is considerably inaccurate to the extent that it is almost unusable for a vertical measurement such as sag. Proposed method describes two different approaches to improve the accuracy of data from a cluster of cheap GPS receivers so that they can be used for sag measurements. Kalman filter and bad data rejection techniques were adapted to reduce vertical error in measurement of sag [3, 4]. An error of ±4.5 m in the raw data was reduced to ±0.45 m after using Kalman filter and to ±0.37 m after using the bad data rejection techniques. Therefore, a cluster of cheaper GPS receivers could be a cost effective alternative system for the measurement of sag in an overhead transmission line conductor.

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## REAL TIME INTELLIGENT LOAD SHEDDING SCHEME BASED ON FREQUENCY MEASUREMENT

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Various faults occurring in transmission lines and generators cause severe imbalance between generation and load. To achieve balanced power supply while maintaining system stability necessitates intelligent load shedding. Conventional methods of load shedding are triggered by under frequency relays and are actuated by circuit breaker. The conventional methods are slow without consideration of system conditions and thus may cause incorrect amount of load shedding. Due to the drawbacks of conventional load shedding techniques, an intelligent load shedding system is necessary to improve the response time and predict the frequency decay. Based on the input data, knowledge of past disturbances and system online conditions, the knowledge base periodically requests computation engine to update the priority list thus ensuring fast and optimal load shedding. Load shedding is planned according to priority levels of loads and distinguishes between critical and non critical loads. The neural network technique is used for early detection of the system disturbances. My research work will demonstrate the need for a modern load shedding scheme and new technology of intelligent load shedding. Different load models as a function of frequency will be developed. New algorithm for intelligent load shedding will be designed and tested through extensive modeling and simulation.

## TIME DOMAIN DIELECTRIC SPECTROSCOPY MEASUREMENT FOR TRANSFOMER INSULATION CONDITION ASSESSMENT

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Dampness and aging of oil-paper insulation are prominent factors to determine the reliability of power transformers. Moisture has detrimental effects on the dielectric integrity and aging rate of the insulation system. The results obtained from the moisture content analysis of oil samples are found to be inconclusive due to the temperature dependence of oil/paper moisture equilibrium. Pressboard samples can also be tested but it is impractical to extract samples from

critical locations of an in-service transformer resulting in inaccurate analysis of insulation condition. Time domain dielectric spectroscopy has the potential to be an on-site dielectric testing technique to determine the conductivity and moisture content of the insulation materials. With this technique, it is possible to distinguish the dielectric properties of oil and paper insulation systems. The purpose of this research is to develop an experimental setup for Polarization and Depolarization Current (PDC) measurement in the HV Lab to study the dielectric properties of aged and new current transformers.

## VERDET CONSTANT OF QUANTUM CONFINED CdS/CdSe NANOPARTICLES IN PHOSPHATE GLASS

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Verdet Constant characterization for phosphate glass samples doped with quantum dots of CdS/CdSe is reported. The enhancement of Verdet constant of phosphate glass samples doped with quantum dots of Ferric Oxide was studied in detail showing the variation of Verdet constant with change in dopant concentration [1, 2]. Also, magneto-optic properties of CdSe, CdTe and CdS quantum dots doped in borosilicate glasses were discussed earlier [3]. In the present study, the doped glass samples having same dopant concentration were treated at different temperatures and their magneto-optic sensitivities evaluated. Doping the higher bandgap glass matrix with lower bandgap semiconductor nanoparticles induces the formation of quantum dots which increase the electron confinement energies upon excitement and magnifies the Faraday rotation angle and hence the Verdet constant of the glass [4]. The measurements showed an increase in Verdet constant of ~30 times that reported of the original undoped phosphate glass [1]. The application of these types of glasses can be done to Magneto-Optic Current transformers (MOCTs), Optic fiber current sensors and Optical Signal Isolators and highly sensitive current detectors [5, 6].

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## PERFORMANCE AND AVAILABILITY IMPACTS OF DATA HOT-SPOTS IN DISK ARRAYS

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Hot-spots in data storage refer to locations in memory that receive higher levels of activity than other areas [1]. This research investigates the impacts of data hot-spots on performance and system availability of disk arrays. Analysis has been performed [2]–[4] validating the notion of a hot-spot. Sikalinda et al [2] found that 60% of the analyzed data was the size of a single block with very low seek distances. We perform experiments on RAID 5 [5] to show quantitatively how hot-spots affect the performance in terms of I/O throughput and availability in terms of mean time to repair, MTTR. We find that for small access workloads, the performance, and system availability, is dominated by the access pattern (read/write), with negligible change due to increases in hot-spot activity. Workloads with larger accesses see a much larger performance and availability impact with increased hot-spot activity.

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## IMPORTED POWER OPTIMIZATION IN MULTI-AREA POWER SYSTEMS WITH PHASE SHIFTERS

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An interconnected power system is made of several areas that can exchange power through tie lines. Some or all of these tie lines are equipped with Phase Shifting Transformers (PSTs). These transformers are widely used for active power flow control. In a multi-area power system operation, an operator within a control area should know the maximum power that can be imported to the area for the best possible operation of the system. The objective of this research is to optimally evaluate the maximum power that can be imported to a particular area and to obtain optimum settings for the PSTs. This research work suggests an optimization technique that employs an extended DC power flow model and linear programming. Instead of using ac power flow algorithm which leads to complex mathematical expressions and complicates the optimization problem, a DC power flow model is used for the systems involving PSTs. The suggested model makes use of Bus Incidence and Cutset loop matrices to derive simple linear expressions that relates the line flows to the phase shifts introduced by the PSTs. Linear Programming is used for the optimization process. The proposed technique is tested for the IEEE standard systems using MATLAB.

## A WAVELET-BASED METHOD TO EXTRACT FREQUENCY FEATURE FOR POWER SYSTEM FAULT/EVENT ANALYSIS

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Frequency is a vital factor for power system operation and protection. This paper is on extraction of frequency feature for fault/event analysis based on wavelet transform (WT) and fractal geometry (FG). The frequency signal is decomposed by WT-based multiresolution analysis (MRA) and a family of wavelet coefficients is obtained. A maxima line is constructed by connecting the maximum point in the wavelet coefficients across all the decomposition levels. A differential box counting (DBC) method based on FG is applied to compute the fractal dimension of the maxima line. It is realized that the feature of a frequency signal can be characterized by a fraction number-fractal dimension. A simulation is carried out in PSS/E to generate different faults in the power system. The proposed algorithm is implemented to extract the features of the faults. The results verify the effectiveness of the proposed method.

## HEV ENERGY MANAGEMENT STRATEGIES USING FUZZY LOGIC

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Fuel Cell-Supercapacitor-Battery Hybrid Power Systems represent a promising architecture to satisfy the energy requirements for road vehicles. The objective of an energy management is to minimize the hydrogen consumption at the same time that the efficiency without compromising the performance of the overall system. In order to achieve these goals, energy management strategies have to be defined. Due to the fact that fuzzy logic control can deal with a considerable amount of variables simultaneously, its use is a reasonable option in order to reach an optimized solution of the energy management problem. In this study, fuzzy logic has been chosen as a tool to implement the control strategies. A simulation environment has been developed in order to test the control strategies, it includes models for the power supply and energy storage devices, the power electronics that comes into play and the energy required from the vehicle.

## SPECTRUM SENSING AND RECONSTRUCTION FOR COGNITIVE RADIO

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The Federal Communications Commission (FCC) opened free 'white space' spectrum on November 4, 2008. In this way, Google and other technology companies that wanted access to more free spectrum have gotten their wish. The prerequisite of the access to the free spectrum is to find this kind of spectrum. This paper deals with spectrum sensing and spectrum reconstruction under the umbrella of cognitive radio which is the smart radio to explore and exploit the free spectrum. Spectrum analyzer is used to emulate cognitive radio to do spectrum sensing. The advantage of equipment-based spectrum sensing is to perform quick and semi-continuous measurements and extract more information about the spectrum under investigation. Total variation (TV) reconstruction method is employed to rebuild the spectrum and find the boundary of the frequency band which is occupied.

## ELECTROMECHANICAL WAVE ANALYSIS THROUGH TRANSIENT MAGNETIC MODELING

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Disturbances in phase angle propagate throughout a power system as electromechanical waves with velocities much slower than that of light. These disturbances can set generator rotors in motion with respect to their synchronous reference frame, causing instabilities that limit the operation capabilities of power networks [1]. Normal techniques studying these transients require large, detailed, computationally expensive models that do not offer a global understanding of the problem. This is the reasoning behind the advent of continuum models which develop partial differential equation (PDE) models of a system that capture the wave nature of frequency disturbances as seen by systems such as FNET (Frequency Monitoring Network) [2]. These approaches currently require the development of schemes such as finite differencing to solve the governing equations. It is the approach of this work to take advantage of the similarities of the continuum equations derived in earlier works to the widely accepted equations of electromagnetism to use the methods of the latter to solve the problems of the former. This enables the application of powerful commercially available electromagnetic software to continuum power system problems. To prove the validity of this method it was applied to a 27-bus system and compared to the results of other continuum and conventional methods. It was shown to be quite comparable and to have distinct advantages. The method is currently being applied to a much larger, 220 bus system.

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## OPTIMIZATION OF AVAILABLE TRANSFER CAPABILITY (ATC) THROUGH STOCHASTIC CONTROL

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A good number of computational tools have been developed for power system engineering and the marketing of electric power system. This task is made more cumbersome following the complexities arising from the deregulation of electric power system. One of the major concerns in contemporary electricity environment is the quantification of the remaining ability of the transmission component to transmit power without violating reliability margins. This remaining capability to transfer power in the physical transmission network for further commercial activity over and above already committed uses has been termed Available Transfer Capability (ATC) by NERC. However, the NERC document did not specify a particular methodology for estimating the ATC. There is a general consensus that load demands have a probabilistic behavior due to the stochastic nature of power systems. Hence, this probabilistic behavior of electric loads indicates that the ATC would behave probabilistically too. In an attempt to appropriately model ATC by incorporating the probabilistic behavioral pattern of power systems, this research is aimed at taking a critical look at the existing electricity market models as well as optimize ATC using stochastic control. When completed, this work will provide efficient tools for the optimal evaluation of ATC, thermal loadability of the line and improved computation efficiency.

## CHARACTERISTICS OF THERMALLY AGED OIL-IMMERSED INSTRUMENT TRANSFORMERS

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The de-regulation process in North-America requires higher indexes of reliability whilst lower costs of operation. Independent power producers, transmission companies, system operators and distribution utilities work to maintain service objectives. Therefore, industry and academics have been together looking for technically feasible procedures to minimize maintenance shutdowns and equipment failure. One of the solutions is to apply Condition-Based Maintenance with reliable diagnostic tools capable to identify ageing or faulty conditions of the electrical equipment. Instrument transformers are an essential component within the electrical system and failure caused by breakdown of the high voltage insulation is usually followed by explosion and fire that may affect other electrical devices and personnel operating nearby. Two non-invasive techniques are being studied at the high-voltage / high-current laboratory at Tennessee Tech University. One is related to the power loss ( ) measurement of the entire insulating system and the second one is based on the analysis of the gas evolution in the liquid insulation. Results of the analysis carried out to date are presented in this document together with a correlation to Loss-of-Life criterion defined by IEEE Standards. Future research work is also described.

## PV – FUEL CELL – ELECTROLYZER MICRO-GRID CONTROL AND OPERATION IN REAL TIME DIGITAL SIMULATOR

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An effective way to realize the integration of distributed generation is to consider it together with the load as a subsystem and thus constitute a micro-grid. One operational advantage is that the micro-grid can be separated form the main grid during system disturbance or fault. Other advantages include higher efficiency of the individual power sources and lower costs. Proper control is needed to maintain micro grid's reliability when additional sources are added and also during disconnections from the main grid. Micro-grid with only green energy sources consisting of Photovoltaic (PV) arrays, fuel cell, supercapacitor and electrolyzer, is modeled and implemented in Real Time Digital Simulator (RTDS) serving a village load. Operating scenarios under fluctuating load conditions using an appropriate control strategy are simulated and analyzed. PV arrays provide power to the village load continuously according to solar radiation. If the power generated by PV is larger than the load demand, the surplus power is supplied to the electrolyzer and store hydrogen. In case the power generated by the PV array is not sufficient to supply the load, the fuel cell converter is controlled to compensate the shortage, while supercapacitor supplies the load transients. The advantages of using RTDS for micro-grid studies are presented. Future work includes optimized control strategy and automatic control between islanding mode and grid-connected mode.

## A NOVEL CACHE DESIGN FOR SSD

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Compared to hard drive, which has an over 40 years history, SSD is new and to some extent, immature. Its excellent random access performance makes it the new star of data storage technology. However, as a member of flash memory family, SSD has some inherent drawbacks, such as limited erasure cycles, low small write performance [1], etc., which are yet to be solved. This research focus on addressing the small write performance problem through an efficient write cache algorithm design. Upon broad investigations [2] [3] on various aspects of SSD, we came up with a write buffer management algorithm which aims at reducing the number of updating requests submitted to SSD, reducing SSD's erasure count and therefor improving the small write performance. Algorithm design and tradeoffs are discussed, and performance analysis based on simulation is given.

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## COMPRESSED SENSING FOR UWB

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The demanding characteristics of the UWB technology include extremely high sample rate in the receiver. These sampling rates require sophisticated devices, sometimes out of the scope of the state-of-art technology. Among the different methods to make the reception possible, Compressed Sensing seems to be the one that presents better performance. It consists basically in compressing the information while this is sampled by avoiding processing a huge chunk of unnecessary data and lowering the sampling rate. In order to reconstruct the data, different methods came up showing different features but presenting the same tradeoff between sampling rate and processing time. Using real measurements of the channel, performance in different environments are analyzed for different frequencies. Thus, this study will help to understand better the Compressed Sensing techniques applied to a real communication, and then decide which method suits better in a given situation.

## MULTIPLE INPUT DC-DC CONVERTER FOR ELECTRIC AND HYBRID VEHICLES

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The proton exchange membrane fuel cells (FCs) are being increasingly accepted as the most appropriate supply for electric vehicles (EVs) because of the clean and efficient energy they offer, without down-grading performance and driving range. To achieve maximum efficiency for the FC system a battery storage unit (BU) can be used as an additional power source. New power electronic converters and control strategies are needed in order to combine two or more on – board generation units and storage units and to improve fuel efficiency, vehicles' performance and driving range. This project aims at building a new multiple input dc – dc converter to combine two power sources in order to

run a power train. Additionally, a control strategy is being developed to achieve highest efficiency of the on-board power sources. The converter circuit together with the control strategy is being implemented in Matlab/Simulink. The current simulation results cover one direction power flow. Next step to be performed is to adjust the controller to bi – directional power flow to allow battery charging during regenerative braking and steady state conditions. After achieving satisfying results the circuit will eventually be built for hardware testing.

# MANUFACTURING AND INDUSTRIAL TECHNOLOGY ENGINEERING
## UNDERGRADUATE STUDENTS

### OPTIMIZING MEASUREMENT ACCURACY OF HYDROGEN GAS POROSITY IN ALUMINUM CASTINGS UNDER VARYING BAROMETRIC PRESSURES

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Hydrogen gas porosity in aluminum castings have long been measured using vacuum and finding the specific gravity by weighing samples in air and in water. Most foundries maintain a set vacuum on the sample as it solidifies, usually -27 inches mercury. Barometric pressure can vary between 27 and 31 inches of mercury, meaning the sample having a gauge reading of -27 in. Hg. has between 2 and 4 inches absolute pressure. The ideal gas law applied to the gas volume says that the gas volume at 4 inches mercury is twice as much at 2 inches. This gives 50% error swing from an average barometric pressure of -30 inches mercury. The scales used in weighing the aluminum samples have minimum accuracy to the 0.1 gram. The specific gravity of degassed aluminum cast under vacuum varies between 2.4 and 2.6, which for a 140 gram sample will give a 2% range of error. It is proposed in this paper to sacrifice accuracy in the weighing of the samples by solidifying at an optimal absolute pressure to minimize relative error. The vacuum required to give the best accuracy of gas porosity is found for degassed aluminum 356 for open top and closed containment samples.

# MECHANICAL ENGINEERING
## GRADUATE STUDENTS

### WETTING BY MOVING TRIPLE LINES

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Collaborator: Dr. Srikanth Vedantam (Department of Mechanical Engineering, National University of Singapore, Singapore)

Wetting is a fundamental phenomenon. The control of wetting behavior on non-ideal surfaces has numerous practical applications. Wettability of solid surfaces is characterized by the contact angle that a sessile drop exhibits on the solid surface. The motion of the triple line is known to play an important role in determining this macroscopic contact angle due to its ability to be pinned at various defect locations on real surfaces. This results in contact angle hysteresis (CAH) on real surfaces. Wetting hysteresis was studied on smooth, chemically heterogeneous surfaces and the effect of the moving triple line kinetics was investigated. A modified Wilhelmy plate apparatus was set up to measure the contact angles and observe the triple line contortions during advancing and receding events. Chemical heterogeneity was introduced to a smooth glass slide in the form of a single stripe of hydrophobic material (silanization of the sample) on a hydrophilic material (glass slide itself). The triple line was observed to readily wet the hydrophilic material and hesitate to wet the hydrophobic material. This study was extended to one and two-dimensional heterogeneities. The work provides insight into the fabrication of chemically heterogeneous surfaces for desired wetting applications.

### THE SHAPE OF A SESSILE DROP

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Hydrophilic and hydrophobic are prevalent terms in the study of the interaction of liquid with a solid surface. Contact angle is an important parameter which characterizes the interaction between the liquid and solid surface. In this study, we investigate the local contact angles and the configuration of the contact line shape of a liquid drop that rests either on a homogenous or heterogeneous solid substrate. We use the numerical algorithm 'Surface Evolver' which is an interactive program for the study of surfaces shaped by surface tension, gravitational and other energies. The algorithm calculates the velocity at each vertex and

the vertex is moved in the direction such that the surface evolves towards a minimum energy. The wetting behavior of liquid drops on periodically structured heterogeneous surface is investigated and a comparison is made with the experimental results available. The shapes and the energies of the drop are computed using the Surface Evolver. The effect of the length scales and pinning of the contact line on the shape of the drop evolved will be investigated.

## EULERIAN MULTIPHASE MODEL
## OF FRAGMENTING FLOWS

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An Eulerian multiphase model is developed to study the fragmentation and transport phenomena in multiphase flow systems. In this model, the range of particle size is divided in to a finite number of size classes with each particle size class being treated as an individual phase. The fragmentation process is modeled using population balance approach. In this approach, the parent particle size classes are encouraged to breakup into any of the daughter particle size classes based on a predefined breakage phenomenology. The accompanying mass and momentum transfer resulting from the fragmentation process are modeled as source terms in the corresponding mass and momentum conservation equations. Further, the breakup of parent particle size class is also made to depend on the local flow parameters such as, Weber number. By employing this methodology in FLUENT, one can model the fragmenting particulate flow system. In here, the developed model is applied to a spray system to study the spatial evolution of daughter particle size distribution.