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golden key to the discovery of new knowledge in all disciplines **TUESDAY APRIL 1 2008** at the Roaden University Center

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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, April 1, 2008

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.

April 1, 2008

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 four consecutive years, one of the Best Southeastern Colleges by the Princeton Review. U. S. New 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,

TOUT A.B

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 2008, 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

### COLLEGE OF AGRICULTURAL & HUMAN SCIENCES

### AGRICULTURE UNDERGRADUATE STUDENTS

EFFECTS OF WASTEWATER DISCHARGE ON PIGEON ROOST CREEK

Kara Tipton Agriculture Faculty Research Advisor: Dr. Janice Branson

Wastewater from approximately 24,000 residents of the city of Cookeville [1] is discharged into Pigeon Roost Creek following treatment at Cookeville Wastewater Treatment Plant. The objective of this study is to determine discharge effects on water quality. Four sites were sampled - one 300 ft. above discharge (PR4), at discharge point (PR3), 1000 ft. below discharge (PR2), and one mile downstream from discharge (PR1). Laboratory analyses included biological oxygen demand (BOD), pH, conductivity, turbidity, and total coliform/E. Coli. Significant changes occurred in pH, conductivity, turbidity, and BOD at PR3. Total coliform did not change at any site, however, E. Coli levels fluctuated slightly. At PR1 all measured parameters were either the same as PR4 or beginning to return to previous levels. Discharge of treated wastewater produced localized effects, but water quality at a distance downstream approaches original levels.

#### Reference

1. http://www.city-data.com/city/Cookeville-Tennessee.html

### HUMAN ECOLOGY UNDERGRADUATE STUDENTS

EFFECT OF FAT SOURCES ON DROP BISCUIT ACCEPTABILITY

Beth Rohling and Ryan Tomlinson Human Ecology Faculty Research Advisor: Dr. Cathy Hix-Cunningham

The purpose of this experiment was to determine the sensory, physical, cost, and nutritional differences of drop biscuits made with three versions of saturated and unsaturated fats. The biscuits made with three ratios of mayonnaise to shortening were compared: 100%:0%, 50%:50%, and 0%:100%. They were evaluated by twenty panelists for color, flavor, texture, and overall acceptability. The drop biscuits were also assessed for air cell distribution, height, cost, and nutritional analysis. After two replications, differences between treatments were minor, although the 100% mayonnaise was preferred slightly more in all categories. Panelists detected little difference in color, flavor, texture, and overall acceptability, which is signified by close replication averages. Nutrient analysis and research suggested 100% mayonnaise was the more healthy fat choice. Although vegetable shortening is a common source of biscuit fat, mayonnaise proved to be an acceptable substitute.

### CHEMISTRY GRADUATE STUDENTS

SYNTHESIS AND CHARACTERIZATION OF POTENTIAL ANTI-CANCER AGENTS: PHENANTHRENEQUINONE THIOSEMICARBAZONE PALLADIUM COMPLEXES

Rachel C. Huxford Chemistry Faculty Research Advisor: Dr. Edward C. Lisic

This work presents the synthesis and characterization of a new series of phenanthrenequinone thiosemicarbazone palladium complexes. One of these complexes, derived from phenanthrenequinone thiosemicarbazone, has previously been described in literature. This complex displayed activity against MCF-7 human breast cancer cells, suggesting that the other complexes are potential anti-cancer agents [1]. The other complexes of this series are derived from phenanthrenequinone methylthiosemicarbazone, phenanthrenequinone ethylthiosemicarbazone, phenanthrenequinone phenylthiosemicarbazone, and phenanthrenequinone benzylthiosemicarbazone. Each tridentate thiosemicarbazone ligand (L), reacted with K<sub>2</sub>PdCl<sub>4</sub>, results in a square planar palladium complex in the form Pd(L)Cl. The complexes were characterized via <sup>1</sup>H nuclear magnetic resonance spectrometry, infrared spectrometry, and UV-Visible spectroscopy, and their magnetic susceptibilities were obtained. The crystal structure of the phenanthrenequinone benzythiosemicarbaone complex in N,N-dimethylformamide is presented.

#### Reference

1. Padhye, Subhash; Afrasiabi, Zahra; Sinn, Ekk; Fok, Jansina; Mehta, Kapil; Rath, Nigam. Inorganic Chemistry Communications. 2005, 44 1154-1156.

THEORETICAL STUDY ON ELECTRON TRANSFER BETWEEN CYTOCHROME B5 REDUCTASE AND CYTOCHROME B5

Sireesha Kollipara Chemistry Faculty Research Advisor: Dr. Scott Northrup

Electron transfer between proteins has attracted considerable experimental and theoretical attention. Studies on electron transfer between proteins strongly support that electrostatic interactions play a major role in protein electron transfer [1]. Cytochrome  $b_s$  reductase catalyses the transfer of electrons from nicotinamide adenine dinucleotide

(NADH) to cytochrome b<sub>5</sub>[2]. Experimental studies on these proteins indicated the presence and involvement of charged amino acid residues like lysine, aspartic, and glutamic acid in the electron transfer reaction [3]. Theoretical modeling studies on these proteins will provide a greater in-depth understanding of the molecular basis of the reaction. We present some preliminary results of Brownian dynamics simulations [4] used to calculate bimolecular rate constants, which can be directly compared to these experiments. Crystallographic coordinates of the proteins have been supplemented with model building of missing residues and assignment of electrostatic partial charges necessary to calculate accurate electrostatic fields around the proteins.

#### References

- 1. Matthew, J., 1985, Electrostatic effects in proteins: Ann. Rev. Biophys. Biophys. Chem, 14, p. 387,417.
- Mauk, A., Mauk, M., Moore, G., and Northrup, S., 1995, Experimental and theoretical analysis of the interaction between cytochrome c and cytochrome b<sub>5</sub>: J Bioeng Biomem, 27, p. 311,330.
- 3. Shirabe, K., Nagai, T., Yubisui, T., and Takeshita, M., 1998, Electrostatic interaction between NADH-cytochrome b<sub>5</sub> reductase and cytochrome b<sub>5</sub> studied by site-directed mutagenesis: Biochim Biophys Acta, 1384, p. 16,22.
- 4. Northrup, S., Boles, J., and Reynolds, J., 1988, Brownian dynamics of cytochrome c and cytochrome c peroxidase association: Science, 241, p. 67,70.

### CHEMICAL FINGERPRINTING ON CLANDESTINE METHAMPHETAMINE BY LC/MS/MS

Sri Bharat Madireddy Chemistry Faculty Research Advisor: Dr. Jeff Boles

Over the years Methamphetamine (N-methyl-1phenylpropan-2-amine), a potent psycho-stimulant, abuse has been a major cause of concern throughout the world, especially in the State of Tennessee.<sup>1</sup> Illicit manufacture of methamphetamine in clandestine laboratories has been carried out with the use of minimal over-the-counter ingredients. [1] The present research is on positive identification of the location of the manufacturing unit by designing a 'signature profile, 'impurity profile' or 'chemical fingerprint' by LC/MS/MS. [2] This is carried out by establishing a database of selected set of impurities by obtaining pure standards of those impurities and later comparing the seized samples with the database for positive identification of the types and quantities of impurities present, the method of synthesis, the proportions, source and purity of starting materials, the reaction conditions, and the purification procedures, if any. The research focuses on developing a method for obtaining chemical profile for clandestine methamphetamine by LC/MS/MS and further

supporting the obtained results by designing a qualitative and quantitative technique using GS/MS/MS.

#### 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)
- 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

EXTRACTION OF CESIUM FROM ALKALINE MEDIA UTILIZING A FUNCTIONALIZED CALIX[4]ARENE-BENZOCROWN ETHER

### John D. Partridge

#### Chemistry

Faculty Research Advisor: Dr. Dale D. Ensor Collaborators: Laetitia H. Delmau, Bruce A. Moyer (Chemical Separations Group, Oak Ridge National Laboratory) Richard Bartsch and Hui Zhou (Department of Chemistry, Texas Tech University, Lubbock, TX)

Selective separation of cesium from other alkali metals under alkaline conditions is a challenging problem in nuclear waste processing. The discovery of calixarene-crown ethers provided a new class of cesium-selective extractants that have been shown to be the strongest and most selective extractants for cesium yet developed. This investigation describes the properties of lipophilic calix[4]arenebenzocrown-6 ethers in the 1,3-alternate conformation functionalized with acidic pendant group containing an anisole substituent (CAB6-anisole). The extraction of cesium from aqueous nitrate solutions into toluene solutions containing the CAB6-anisole was measured as a function of pH, extractant concentration, and nitrate concentration. These distribution values were mathematically modeled to determine the formation constants of the complexes formed in the organic phase. The resulting formation constants showed that attachment of the acid group to the calixarenecrown molecule reduced the binding stability for the cesium ion upon contact with an acidic solution. These results will be compared to previous work and the application of these compounds to cesium separation processes will be discussed.

### CHEMISTRY UNDERGRADUATE STUDENTS

ANALYSIS OF EMERGING CONTAMINANTS IN WASTEWATER TREATMENT PLANT EFFLUENT BY GC-MS/MS

Marki Carlisle Chemistry Faculty Research Advisor: Dr. John Harwood

The purpose of this research is to analyze the presence of endocrine disrupting compounds in samples of water and sediment from a stream near a local Wastewater Treatment Plant. These compounds are important to study because of the physiological effects they could have on the population. Research has shown that these compounds can imitate natural hormones in animals and could even be toxic if one is exposed to enough of these compounds [1]. The two compounds chosen to detect for are Triclosan and Galaxolide. Triclosan, an anti-bacterial and anti-fungal agent, and Galaxolide, a synthetic musk, are commonly used in Personal Care Products distributed globally [2]. Samples of water and sediment will be obtained from upstream and downstream of Pigeon Roost Creek near the Wastewater Treatment Plant in Putnam County, Tennessee. These samples will be analyzed using tandem GC-MS/MS with MRM to achieve highly sensitive results.

### References

- 1. "On-site solid phase extraction and laboratory analysis of ultra-trace synthetic musks in municipal sewage effluent using gas chromatography-mass spectrometry in the full scan mode." Osemwengie, L.I., Steinberg, S. Journal of Chromatography A, 2001, 932, 107-118.
- "Broad range analysis of endocrine disruptors and pharmaceuticals using gas chromatography and liquid chromatography tandem mass spectrometry." Trenholm, Rebecca A., Vanderford, Brett J., Holady, Janie C., Rexing, David J., Snyder, Shane A. Chemosphere, 2006, 65, 1990-1998.

### THE ALDOL CONDENSATION OF ACETOPHENONE WITH ALDEHYDES AND KETONES

Aileen Guerrero and Dan Roubik Chemistry Faculty Research Advisor: Dr. Daniel J. Swartling

Acetophenone was reacted with various aldehydes to give the corresponding Aldol condensation products in very good yield. The products were characterized by NMR spectroscopy and their physical properties measured. The

aldol products will be used in Michael addition reactions with nitromethane to give after several steps analogs of gamma-amino acids, which might possess biological activity.

SYNTHESIS AND CHARACTERIZATION OF A NEW SERIES OF 5-FORMYL-2-FURAN SULFONIC ACID SODIUM SALT THIOSEMICARBAZIDE COMPOUNDS

Erik Hoy, Rachel Huxford, and Erica Stoner Chemistry Faculty Research Advisor: Dr. Edward C. Lisic

This work will present the synthesis of a new series of 5formyl-2-furan sulfonic acid sodium salt thiosemicarbazide compounds. A total of eight compounds: 4-methylthiosemicarbazide, 4-ethyl-3-thiosemicarbazide, 4phenyl-3-thiosemicarbazide, 4-benzyl-3-thiosemicarbazide, thiosemicarbazide, 4-phenylthiosemicarbazide hydrochloride, 4,4-bimethyl-3-thiosemicarbazide, and semicarbazide hydrochloride were combined with 5-formyl-2-furan sulfonic acid sodium salt to synthesize a new series of eight compounds. The compounds were characterized via

#### References

1H NMR.

- 1. "On-site solid phase extraction and laboratory analysis of ultra-trace synthetic musks in municipal sewage effluent using gas chromatography-mass spectrometry in the full scan mode." Osemwengie, L.I., Steinberg, S. Journal of Chromatography A, 2001, 932, 107-118.
- 2. "Broad range analysis of endocrine disruptors and pharmaceuticals using gas chromatography and liquid chromatography tandem mass spectrometry." Trenholm, Rebecca A., Vanderford, Brett J., Holady, Janie C., Rexing, David J., Snyder, Shane A. Chemosphere, 2006, 65, 1990-1998.

### INVESTIGATION OF COFACTOR REACTION(S) IN THE PLP $\beta \text{CA}$ KINETIC ASSAY

Taylor King Chemistry Faculty Research Advisor: Dr. Jeff Boles

Tryptophan Synthase (TS) is a bifunctional, tetrameric, and Pyridoxal-5'-Phosphate (PLP) dependent enzyme which catalyzes the last two steps in the biosynthesis of L-Tryptophan. TS is just one of the numerous enzymes broadly used in biochemical studies. The enzyme plays a critical role in synthetic organic chemistry and has received increased attention in the past decade. TS is widely used as a model in substrate channeling and protein-protein interaction studies, and in the production of novel L-Tryptophan analogs (Miles, 1995). Recently, a problem with the TS spectrophotometric

assay was discovered (Henderson, 2001). The formation of Tryptophan by TS is monitored as an increase in absorbance at 290nm. Previous research discovered that in the absence of enzyme, a considerable increase in the absorbance at 290nm is noted. The non-enzymatic reaction occurs in various buffers, pH values, and varying concentrations. This poster seeks confirm that the increase in absorbance at 290nm is due to a reaction between β-Chloro-Alanine and PLP as was first suggested by previous researchers (Henderson, 2001 & Fortenberry, 2005). The use of liquid chromatography mass spectrometry mass spectrometry has revealed insight into the products formed by the reaction of these compounds. The proposed mechanisms explain how pyruvate is formed during the course of this reaction (Fortenberry, 2005), and this has been confirmed through experimentation. These non-enzymatic reactions that occur concurrently with enzymatic assays have far reaching implications in the biochemical community. Researchers have noted problems throughout the years but they were never able to explain what was seen in the laboratory (Gregerman, 1956). The aim of this research is to make light of the problems associated with PLP-dependant enzymes such as TS and potentially minimize their detriment to future research.

### SYNTHESIS AND CHARACTERIZATION OF NQSA THIOSEMICARAZONE COMPOUNDS

Kelly Monteen and Megan 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 will also be described.

### KNOEVENAGEL COUPLING OF MELDRUM'S ACID WITH ALDEHYDES AND KETONES

Dan Roubik and Casey McCormick Chemistry Faculty Research Advisor: Dr. Daniel J. Swartling

Meldrum's acid was prepared from malonic acid and acetone in moderate to good yield. The prepared acid was used in reactions with various aldehydes and ketones to give the corresponding Knoevenagel condensation products in good yield. The products were characterized by NMR spectroscopy and their physical properties measured. The Knoevenagel products will be used in Michael addition reactions with nitromethane to give after several steps analogs of gammaamino acids, which might possess biological activity.

### COMPARISON OF A SERIES OF PHENANTHROLINEQUINONE THIOSEMICARBAZONE COMPOUNDS

Keith Steelman and Erica Stoner Chemistry Faculty Research Advisor: Dr. Edward C. Lisic

Condensations of ketones and semicarbazides to form semicarbazones is a common organic synthesis has been studied for many years. Thiosemicarbazones have fewer limitations due to their ability to complex with both soft and hard acids, including many of the later transition metals. Thiosemicarbazones attached to polycyclic compounds are additionally useful because of the visible color change that they undergo in the presence of metal ions in solution. Phenanthrolinequinone thiosemicarbazones are interesting since they are bifunctional because of the presence of the pair of nitrogens at the back of the ring system. These provide an additional bidentate binding site beyond the multidentate binding of the thiosemicarbazone "arm". This presentation describes the synthesis and characterization of some new phenanthrolinedione-thiosemicarbazone compounds.

### SYNTHESIS AND CHARACTERIZATION OF NEW CHROMONE THIOSEMICARBAZONE COMPOUNDS

Erica L. Stoner and Rachel C. Huxford Chemistry Faculty Research Advisor: Dr. Edward C. Lisic

Thiosemicarbazone compounds are potent biological agents [1, 2], and also act as ligands to a whole host of transition metal ions such as palladium and nickel [3-5]. A series of eight new thiosemicarbazone and semicarbazone compounds synthesized from a formyl chromone backbone in our laboratory will be presented. The synthesis of this new series of compounds is straightforward, and characterization by <sup>1</sup>H NMR and IR supports the proposed structures. Research efforts to synthesize the palladium complexes will also be discussed.

### References

- 1. Padhye, S. Coordination Chemistry Reviews. 1985, 63, 127-160.
- 2. West, Douglas X.; El-Sawaf, Ayman K.; Bain, Gordon A. Transition Metal Chemistry (1998), 23(1), 1-6.
- Afrasiabi, Zahra; Sinn, Ekkehard; Chen, Junnan; Ma, Yinfa; Rheingold, Arnold L.; Zakharov, Lev N.; Rath, Nigam; Padhye, Subhash. Inorganica Chimica Acta. 2004, 357, 271-278.
- 4. Afrasiabi, Zahra; Sinn, Ekk; Lin, Weisheng; Ma, Yinfa; Campana, Charles; Padhye, Subhash. Journal of Inorganic Biochemistry. 2005, 99, 1526-1531.

5. Padhye, Subhash; Afrasiabi, Zahra; Sinn, Ekk; Fok, Jansina; Mehta, Kapil; Rath, Nigam. Inorganic Chemistry Communications. 2005, 44, 1154-1156.

### COMPUTER SCIENCE GRADUATE STUDENTS

### ANNOTATING DIGITAL DOCUMENTS FOR IMPROVED SEARCH RESULTS IN A DOCUMENT REPOSITORY

Michael Baldwin Computer Science Faculty Research Advisor: Dr. Michael Rogers

Since annotation is already one of the most commonly occurring activities involving digital documents [1] there is potentially a large amount of extra, user added, information that could be used to improve provide more powerful and accurate searching methods. This work seeks to develop the technologies, including an annotation tool and a specialized document repository, needed to demonstrate this capability. The annotation tool will allow a user to produce XML standoff markup, i.e. markup stored separately from the original document, [2] which will be stored in the repository along with the document. By utilizing a distributed document annotation process many users can annotate documents for submission to a single central repository. This document repository can then use the user submitted metadata to provide more powerful and flexible searching. Search queries can be specified using traditional keyword based approaches or by more powerful query languages such as XPath and XQuery.

### References

- A. J. B. Brush, D. Bargeron, A. Gupta, and J. J. Cadiz, "Robust annotation positioning in digital documents," in CHI '01: Proceedings of the SIGCHI conference on Human factors in computing systems. New York, NY, USA: ACM, 2001, pp. 285–292.
- Thomas, P. L., and Brailsford, D. F. Enhancing composite digital documents using xml-based standoff markup. In DocEng '05: Proceedings of the 2005 ACM symposium on Document Engineering (New York, NY, USA, 2005), ACM Press, pp. 177-186.

### AN INVESTIGATIVE STUDY OF BUFFER EXPLOITS FOR CLOSER ANALYSIS OF SECURITY BREACHES

### Rob Dye

Computer Science Faculty Research Advisor: Dr. Ambareen Siraj

Stack and buffer overrun exploits account for a large number of the security vulnerabilities that are reported each year. According to the United States Computer Emergency Readiness Team (CERT), over half of the top 20 most severe vulnerabilities have been related to these kinds of weaknesses [1]. Techniques for exploiting such vulnerabilities include stack smashing, heap smashing, arc injections, and pointer subterfuge [2]. This research will investigate modern approaches and tools available for creating various kinds of overrun exploits and compare them with the tools that have been used by hackers in the past. Additionally, techniques will be discussed for detecting and eliminating buffer overrun weaknesses before they can be exploited for possible security breaches.

#### References

- 1. US-Cert Vulnerabilitiy Notes by Metric; http://www.kb.cert.org/vuls/bymetric?open&start=1&co unt=20
- 2. Pincus, J.; Baker, B.; "Beyond Stack Smashing: Recent Advances in Exploiting Buffer Overruns", Security & Privacy Magazine, IEEE, Volume 2, Issue 4, Jul-Aug 2004 Page(s):20-27

### SECURITY ANALYSIS OF DATA DISSEMINATION IN WIRELESS SENSOR NETWORKS

Jeremy Langston Computer Science Faculty Research Advisor: Dr. Ambareen Siraj

The latest movement in sensory data collection uses wireless communications. Usage of wireless communications lends itself to lower costs in installations (e.g. labor, copper/fiber media) and allows the sensor locations to be more easily relocated. However, using an open medium in wireless data relay raises security issues [1], [2]. Since each sensor node is typically resource limited, the transmission range is also limited and, thus, data must hop from one node to the other [3]. This research looks at the problems with the transfer of data between sensor nodes from the security aspects such as confidentiality, integrity, and availability.

#### References

1. G. A. Yong Wang and B. Ramamurthy, "A survey of security issues in wireless sensor networks," IEEE Communications Surveys and Tutorials, vol. 8, pp. 2–23, Apr. 2006.

- S. Ravi, A. Raghunathan, P. Kocher, and S. Hattangady, "Security in embedded systems: Design challenges," Trans. on Embedded Computing Sys., vol. 3, no. 3, pp. 461–491, 2004.
- M. Shao, S. Zhu, W. Zhang, and G. Cao, "pDCS: Security and privacy support for data-centric sensor networks," in INFOCOM 2007: Proceedings of the 26th International Conference on Computer Communications. IEEE, 2007, pp. 1298–1306.

INCORPORATING VISUALIZATION IN AN INTERPRETED LANGUAGE FOR EDUCATIONAL BENEFIT

Brandon Malone Computer Science Faculty Research Advisor: Dr. Frank Hadlock

While the notion of employing animation and visualization to intuitively explain algorithm behavior dates back to the '80s [1], the educational benefit of these visualizations remains largely untapped. Recent research into the utility of algorithm visualizations cites four key paradigms in educationally effective visualizations: responding, in which students answer questions about upcoming and past behavior; changing, in which students provide input to cause desired algorithm behavior; constructing, in which students create their own visualization; and presenting, in which students explain the algorithm with the visualization as an aid [2]. This research investigates an interpreted programming language which espouses these paradigms by providing primitive constructs to simplify the creation and presentation of educationally effective visualizations.

#### References

- 1. Marc H. Brown. Algorithm Animation. MIT Press, Cambridge, Massachussets, 1988.
- Naps, Thomas L., JHAVE Addressing the Need to Support Algorithm Visualization with Tools for Active Engagement. IEEE Computer Graphics and Applications. 2005.

### TOOLS AND TECHNIQUES FOR SSE-CMM IMPLEMENTATION

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

With the immense popularity of globalization and distributed systems, the need for standardization of organization wide security practices has become a high priority. Different studies have shown that organization-

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wide standardization of practices increases productivity [1], efficiency, and customer satisfaction. The Security System Engineering Capability Maturity Model (SSE-CMM) offers industry practitioners such a choice of security engineering standard that can be implemented and integrated at different organizational levels according to assurance needs [2]. Although SSE-CMM provides the necessary roadmap for adopting organization wide quality security engineering practices, it does not specifically point out any tools and techniques that can be used to help reach the goals described in the standard. This research provides insight to security practitioners about availability of possible tools and techniques that would aid them in implementing the recommended guidelines described in SSE-CMM to adopt the standard organization wide.

#### References

- 1. Herbsleb, James et.al. Benefits of CMM-Based Software Process Improvement: Initial Results. Software Engineering Institute, Carnegie Mellon University. 2007
- Hefner, Rick et.al. "The Systems Security Engineering CMM." The Journal of Defense Software Engineering. Oct. 2005

### TOWARDS A UNIFYING TAXONOMY FOR INFORMATION ASSURANCE MEASURES AND METRICS

Emily Sherrill Computer Science Faculty Research Advisor: Dr. Ambareen Siraj

Information assurance (IA) is the term applied to the confidence that one has in a system's ability to maintain the confidentiality, integrity, and availability of data [1]. The measures and metrics needed to determine the level of IA often differs from system to system according to its assurance needs. This research will analyze some of the various forms of IA measures and metrics used by security practitioners. Because the IA metrics will often differ, taxonomies have been developed to assist in describing the characteristics of the metrics [1]. The existing taxonomies developed by researchers in this field will be critiqued to identify their strengths and weaknesses. Based on these findings, recommendations will be made towards creating a unifying taxonomy.

### Reference

 J. Rayford B. Vaughn, R. Henning, and A. Siraj, "Information assurance measures and metrics" state of practice and proposed taxonomy," in HICSS '03: Proceedings of the 36th Annual Hawaii International Conference on System Sciences (HICSS'03) - Track 9, (Washington, DC, USA), p. 331.3, IEEE Computer Society, 2003.

### COMPUTER SCIENCE UNDERGRADUATE STUDENTS

### DEVELOPING A PACKET SNIFFER USING A LINKSYS WRT54GL ROUTER

Jonathan Borden Computer Science Faculty Research Advisor: Dr. Ambareen Siraj

This research project will be developing a packet sniffer using the Linksys WRT54GL router that will be able to capture packets on a wired and wireless network. Packet sniffing is the interception of raw network data without the originator having knowledge [1]. Packet sniffing can be done using a traditional computer, however, using a modified router provides some distinct advantages. First, the packet sniffing device can be left in an area for extended periods of time allowing it to capture large amount of information. Secondly, since the device will not be aesthetically modified, it will be rather inconspicuous if placed in the right location. In order for the WRT54GL to sniff packets, OpenWRT Linux [2] will need to be installed on the device.

#### References

1. http://www.tech-faq.com/packet-sniffer.shtml 2. http://openwrt.org/

> OPTIMIZATION TECHNIQUES FOR THE FELLEGI-SUNTER MODEL OF RECORD LINKAGE

Ben Eckart Computer Science Faculty Research Advisors: Dr. Doug Talbert and Dr. Ambareen Siraj

The standard statistical model for record linkage for nearly half a century has been the Fellegi-Sunter model [1]. In this approach, record-pairs are given weights based upon the conditional probabilities of the comparison vector occurring given both match and non-match status. The validity of the model is dependent on the assumption that reasonably nonbiased conditional probabilities can be found. This research discusses a way to directly find optimal parameters for the Fellegi-Sunter statistical model of record linkage, using a system of nonlinear equations derived from frequency counts appearing in the data. The equations are tested in both a simulated environment and on real Memphis-area hospital patient records. The benefits and limitations of the equations are reviewed and compared specifically to the method of Expectation Maximization [2].

#### References

- 1. I. P. Fellegi and A. B. Sunter, "A theory for record linkage," Journal of the American Statistical Association, vol. 64, no. 328, pp. 1183–1210, 1969.
- A. P. Dempster, N. M. Laird, and D. B. Rubin, "Maximum likelihood from incomplete data via the EM algorithm," Journal of the Royal Statistical Society. Series B (Methodological), vol. 39, no. 1, pp. 1–38, 1977.

### DYNAMICALLY MAXIMIZING THE PERFORMANCE OF LARGE DATA TRANSFER OVER DEDICATED NETWORK LINKS

Ben Eckart

Computer Science Faculty Research Advisor: Dr. Xubin He (Electrical and Computer Engineering)

New networks are emerging for the purpose of transmitting large amounts of scientific data among research institutions quickly and reliably [1]. These networks only marginally resemble the characteristics of the Internet, rendering the established Internet protocols ineffective. Recent methods have been developed to circumvent these problems, including new protocols which implement both reliable (TCP) and unreliable (UDP) data transfer algorithms [2-6]. Building faster networks and better protocols, however, does not necessarily result in better performance when the end-systems involved are unable to support such speeds. It is therefore necessary to build a protocol adaptive the performance of each system. This research develops such a protocol, Performance Adaptive UDP (PA-UDP), which aims to dynamically maximize performance under many system environments. A mathematical model and related algorithms are proposed that describe the theoretical basis behind effective buffer and CPU management. A prototype based on the PA-UDP architecture is implemented by monitoring the hosts during the data reception period and adjusting to the theoretically optimal rate. Experiments show that PA-UDP outperforms other high-speed protocols.

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### DESIGN AND DEVELOPMENT OF JADE: AN EXPERIMENTAL PROGRAMMING LANGUAGE

Russell J. Royer Computer Science Faculty Research Advisor: Dr. Ambareen Siraj

This research addresses the design and development of an experimental programming language that would combine logical/declarative syntax with imperative programming by integrating a logical database and embedded logical queries with a natural, imperative syntax. It will also explore the nature of such a language using Chinese characters as a syntactic medium. Instead of concentrating on the native syntax and lexicon of Chinese as a natural language, this research will seek to demonstrate the tremendous flexibility that such a medium could present in declaring logical relationships by taking advantage of the explicit nature of some characters and words, and perhaps even the more fundamental nature of the characters themselves (radicals, reused strokes, etc). Such a language would allow both declarative and imperative calls using Roman characters or Chinese characters, and would be structurally and syntactically similar to many modern declarative and imperative languages.

### EARTH SCIENCE UNDERGRADUATE STUDENTS

### COMPARISON OF FLUID CHARACTERISTICS FROM A FAULT ZONE AND MARGINAL FORELAND BASIN

Phillip Derryberry and James Kimbrell Earth Sciences Faculty Research Advisor: Dr. Michael Harrison

Calcite veins from the Sequatchie Valley Thrust zone in middle Tennessee were collected to characterize the geochemistry and temperature of fluids associated with Alleghanian deformation. Specifically, fluid inclusions within the calcite veins were analyzed with a USGS-style heating

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and cooling stage to assess the temperature of homogenization (TH) and the last-ice melting temperature (TM). For veins collected from the Bangor Limestone next to the fault zone, the TH ranges from 55°-205° C and shows a bimodal distribution with modes of 60° C and 120° C. Veins collected from Gordonsville, TN ~110 km to the northwest also show a bimodal distribution of TH, but with modes of 105° C and 120° C. For the TM, the Bangor samples show a mode of 1.5° C whereas the Gordonsville samples show a mode of -18° C, suggesting different fluid sources. Hydrocarbons were detected in the inclusions from both sample sites.

### APPLICATION OF GIS ON THE DISTRIBUTION OF FOSTER HOMES IN THE UPPER CUMBERLAND AREA

Whitney Fuquay Earth Sciences Faculty Research Advisor: Dr. Peter Li

The goal of this project is to show how the integration of GIS into the foster care program provided by the Department of Children Services (DCS) can create highly organized and highly assessable data to insure the accurate and most beneficial placement of the children in their care. The study area of this project is the Upper Cumberland region of Tennessee which includes Cannon, Clay, Cumberland, DeKalb, Fentress, Macon, Overton, Pickett, Putnam, Smith, Van Buren, Warren, and White counties. A range of data analysis will be performed using ArcMap and its various extensions including network analyst. Data will be supplied by the DCS and will be analyzed along with available spatial data and data created for the study area. A successful placement is one in which a child improves or is placed back into their original home. The objective is to determine if successful placements can be attributed to the spatial location of the resource home. The digital maps produced will provide DCS workers the ability to have a more visible understanding of the area they are working in and to better analyze spatial conditions and options that are available for the placement of the child they are working to help. Maps will be produced displaying the counties of the Upper Cumberland region along with the location of resource homes in each county cluster and the distribution of children currently in the care of the DCS.

### APPLICATIONS OF GIS IN THE OIL AND GAS INDUSTRY IN TENNESSEE

Will Goodwin Earth Sciences Faculty Research Advisor: Dr. Peter Li

This research project hopes to begin to fulfill the growing demand for a geographical information system solution

for the existing and future oil and gas wells of the state of Tennessee. Information gathered and analyzed includes but is not limited to spatial, production, operator, and geologic information. Some explored uses for the system are the implementation of an emergency response system through network analysis, matching unknown wells to legal information using gps coordinates, and mapping of underground geologic formations based on location for area specific analysis and future exploration. Overton County is used to show County specific detail such as elevation modeling and orthophotography.

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### PUTNAM COUNTY REZONING USING GIS

Brent Richey Earth Sciences Faculty Research Advisor: Dr. Peter Li

My project corrects the current problem at hand by consolidating students in Putnam County and making school reassignments that best fit the need of the schools, the student, and the community. Using various applications and techniques, it was shown that the problem(s) can be corrected in a manner that is reasonable, fair, and efficient. The impacts of a nonexistent school zoning policy were brought to attention and examined to the point that a need for a school zoning policy is evident. I compiled several charts and used visual simulators to present this need. In addition an approach using computer language code called BASIC, a program was written that balanced school populations based on school capacities. School zones were set up for all seventeen schools in the county, assignments were made that easily displayed where each individual student must attend his or her institution, and impacts to the environment due to unnecessary miles driven were calculated. This study is important because of the inevitability that Putnam County will have little future choice but to soon adopt a school zoning policy to prevent a school overcrowding crisis as the county continues to grow at a rate to an approximation of 3.9% per year.

#### References

TNGIS.org
 Putnam County 911 Emergency Service
 ESRI
 Putnam County School Board

MICRO- AND MESOSCALE STRUCTURES ASSOCIATED WITH THE SEQUATCHIE VALLEY THRUST, TENNESSEE

Matt Silvey and Drew Griswold Earth Sciences Faculty Research Advisor: Dr. Michael Harrison

Numerous mesoscopic-scale shortening structures (faults, folds, and stylolites) are observed in the Upper Mississippian Bangor Limestone within Brown Gap Quarry adjacent to the Sequatchie Valley Thrust in middle Tennessee. These structures trend 020° and 050°, sub-parallel to the strike of the Sequatchie Valley Thrust. The direction of horizontal shortening indicated by these structures (306-316°) is consistent with the shortening direction of the Sequatchie Valley thrust, about 305°. This shortening is also observed at the grain scale. Finite-strain Fry analysis of carbonate grainstone from the quarry and from the Monteagle Limestone near Crab Orchard, TN shows a shortening direction of ~300° and a strain ratio of 1.2-1.3. Pressure solution was an important mechanism that accommodated the shortening.

### MATHEMATICS GRADUATE STUDENTS

NUMERICAL SIMULATION OF GROUNDWATER FLOW

Che Ngufor Mathematics Faculty Research Advisor: Dr. Sabine Le Borne

The goal of this research is to develop effective and efficient iterative solvers for linear problems arising from the discretization of equations governing the flow of groundwater in porous media. We approximate the actual groundwater system by a mathematical model and a computer model numerically solves the mathematical equations. The simulation is performed by sequential decoupling of the flow equation through the Darcy equation producing a dual mixed system. An efficient implementation of a discretization based on the lowest order Raviart-Thomas mixed finite elements technique leads to a saddle point system. Two methods are implemented for solving the saddle point system to yield the unknown velocities and pressures: (1) Using direct linear solvers like MATLAB, (2) using a new and efficient iterative solver we have developed based on the so-called hierarchical matrices. We then visualize the flow field and distribution of heads for both simple and complex geological formations.

### MATHEMATICS UNDERGRADUATE STUDENTS

2-DIMENSIONAL VISUALIZATION OF VELOCITY FIELDS

Edmond B. Smith Mathematics Faculty Research Advisor: Dr. Sabine Le Borne

We have all heard the saying "a picture is worth 1,000 words." This applies such that vectors are worth more than one billion numbers when describing fluid flow. In this research, we use vectors to represent fluid particles' velocities. Each particle has it's own attributes such as: movement in different directions or varying velocities. For many particle systems, it is more sufficient to use vector fields to represent groups of particles. Vector fields allow us manipulate and restrict system as a whole. My research has been to visually show these vector fields by programmed arrows, which allows changing lengths, angles, and origins based on data given for each vector. In the future others will be able to use these arrows printed on a page to interpret how fluids represented by vector fields behave rather than trying to study the trends of numbers. Visual results of research will be presented.

### DOMAIN TRIANGULATION TO APPROXIMATE A 2-DIMENSIONAL DISK

Quinton Westrich Mathematics Faculty Research Advisor: Dr. Sabine Le Borne

In order to run computer simulations which model the dynamics of fluids inside a shape, called a domain, the first step is to program the domain. In practice, we approximate the boundary of the domain with a polygon and then divide the interior of the polygon up into simpler shapes, such as triangles in 2D and tetrahedra in 3D---a process is called triangulation. Many objects we use daily, such as water pipes, engine pistons, and hoses, are nearly circular in two of their dimensions. My project is the triangulation of a 2D disk. Written in the C language, our code arranges triangles so that symmetries simplify and speed up storage and access of the grid points. Numerical data are presented which illustrate this. The next step will be the incorporation of this 2D disk into 3D codes for a wider range of applications.

## COLLEGE OF EDUCATION

### TRIANGULATION OF 3D CUBES FOR COMPUTATIONAL FLUID DYNAMICS

William Wilhoite Mathematics Faculty Research Advisor: Dr. Sabine Le Borne

Computational fluid dynamics, or CFD has applications in fire fighting, air conditioning, and many other fields which are beneficial to society. So far computer triangulations of two dimensional domains have been made for our applications, but no three dimensional domains have been developed. We are making a computer model describing discrete points and sub-polygons of a cube for applications in CFD. We are writing a program to create a text file which describes points, lines, triangles, and tetrahedrons which subdivide of a unit cube. This will allow for approximations in three dimensional domains. Numerical results will be presented.

### CURRICULUM AND INSTRUCTION GRADUATE STUDENTS

PEER INFLUENCES, ATHLETICS, AND FACTORS OF FRESHMEN COLLEGE CHOICE

George Chitiyo Curriculum and Instruction Faculty Research Advisor: Dr. David Larimore

This study was conducted at a four year public university in the south eastern United States during the spring 2007 semester. Data were collected from a sample of 216 freshmen, 78 of whom were athletes. The overall response rate for the survey was 76%. A survey instrument was administered to investigate factors that influenced the freshmen students' college choice, especially peer influences and athletics. A factor analysis was conducted in addition to descriptive statistics. Overall, the most important variables influencing the college choice of high school graduates were those associated with the factor named institutional image. The other factors are: peer influences, high school counselors and teachers, athletic factors, family influence, and spiritual guidance at the university. These factors collectively accounted for 77.3% of the variance in college choice.

### EXCEPTIONAL LEARNING GRADUATE STUDENTS

EFFICACY OF PEER-MEDIATION FOR PROMOTING SOCIAL INTERACTIONS AMONG YOUNG CHILDREN WITH AUTISM Jie Zhang Exceptional Learning Faculty Research Advisor: Dr. John J. Wheeler

The purpose of this research was to investigate the efficacy of peer-mediations for promoting social interactions among young children under 8 years of age diagnosed with autism. A meta-analysis using single-subject studies was conducted with 45 studies from 19 journals between 1977 and 2006. The efficacy of the interventions was analyzed according to the variables that may affect the interventions, including the target children's characteristics, interventionists' characteristics, and intervention features. Inter-rater reliability was determined through doublecoding the variables by the researcher's doctoral advisor. Allison and Gorman's [1] method was used to calculate the effect sizes in order to take trend into account. One-sample t test was used to determine whether the overall effect sizes were significantly different from zero. One-way ANOVA, independent-samples t test, or Tukey's post hoc test were used to compare each effect size within every variable to see whether there was any significant difference.

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### STATISTICAL COMPARISONS OF EFFECT SIZES OF PEER-MEDIATIONS FOR YOUNG CHILDREN WITH AUTISM

Jie Zhang and George Chitiyo Exceptional Learning Faculty Research Advisor: Dr. John J. Wheeler

The purpose of this research was to investigate the differences among effect sizes calculated using three different methods, of peer-mediated interventions for promoting social interactions among young children under eight years of age diagnosed with autism. Allison & Gorman's regression-based method [1], percentage of nonoverlapping data (PND) [3] and d [2] were used to calculate the effect sizes for each child. The effect sizes were computed from data used in a meta-analysis comprising of 45 single-subject studies from 19 journals between 1977 and 2006. In addition to the calculated between PND, d, and the regression-based effect sizes in order to determine the extent of agreement among them.

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### CHEMICAL ENGINEERING GRADUATE STUDENTS

### ADAPTIVE NUMERICAL INTEGRATION OF LITHIUM-ION BATTERY MODELS

Mounika Arabandi

**Chemical Engineering** 

Faculty Research Advisor: Dr. Venkat Subramanian Collaborator: Dr. Vijayasekaran Boovaragavan (Chemical Engineering)

Modeling lithium-ion batteries involves ten partial differential equations in three domains and two dimensions. Finite difference discretization [1] of battery models in spatial coordinates results in 5000 Differential Algebraic Equations (DAEs). For online control, optimization and parameter estimation, there is a need to develop a code that will run in real time (milliseconds). In the literature, typically adaptive time stepping solvers have been reported for many numerical schemes (Runga-Kutta). But, the algorithm for adaptive stepping depends on the numerical methods used. Carefully designed adaptive algorithms have a most significant impact on computational stability and reliability. For batteries, special stiff equation solvers are needed for efficiency. In order to solve DAEs efficiently, we propose to develop new strategies for adaptive time stepping. The efficiency of these solvers will be compared with the existing solvers [2] in the literature.

### References

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### A NOVEL MONTE-CARLO STRATEGY FOR EVALUATING CATHODE MATERIALS FOR LITHIUM ION BATTERIES

### Vinten D. Diwakar

**Chemical Engineering** 

Faculty Research Advisor: Dr. Venkat Subramanian Collaborator: Dr. Harinipriya Seshadri (Chemical Engineering)

A novel simulation strategy is formulated to study the performance of cathode materials in Li-ion batteries. The

methodology [1] takes into account both micro scale properties and macro scale properties. For example, diffusion of spherical electrode particle within the cathode and solvation effects, diffusion coefficients, concentration gradient to determine the diffusion of Li+ within the separator. The electrode particles move in each step to its nearest neighbor distance, employing the random number condition ir(j)>=exp(-dLi1/ds), where 'ir' represents the random number, dLi1 is the nearest neighbor distance for Li<sup>+</sup> in the absence of solvent and ds being the thickness of the solid phase. The second random number criterion is ir(j) > = exp(-dLi1/ds2), dLi1 being the nearest neighbor distance Li<sup>+</sup> can move in the presence of solvent and ds2 being the thickness of the separator. The discharge behavior for LiCoO<sub>2</sub> and LiFePO<sub>4</sub> as cathode materials is in quantitative agreement with existing literature [2, 3].

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### AGGREGATION OF NANOPARTICLES USING REAL-TIME HIGH TEMPERATURE X-RAY DIFFRACTION

James B. Fox Chemical Engineering Faculty Research Advisor: Holly Stretz Collaborators: Andrew Payzant and Roberta Meisner (Oak Ridge National Laboratory)

Real-time X-ray diffraction has been used to determine the changes in structure and morphology of nanocomposites under high temperatures. Polybond X5140/Nanomer I-44P (5% w/w) was compounded at 190°C for 10 minutes, injection molded into small bars, milled to 1mm thickness, and cut into dime size samples. The samples were examined in parallel beam geometry using Cu K a 1 radiation. The composites and pure organoclay did not show a change in the d<sub>oo1</sub> over the entire range of temperatures examined. An additional study was conducted to determine the effects of pressure on organoclay. Cloisite 20A was pressed at 250°C and 6.9 kPa for various lengths of time, and examined using X-ray diffraction. The d<sub>001</sub> of Cloisite changes under these conditions, but the  $d_{101}$  does not change indicating a possible change in space group. Future work includes TEM analysis in conjunction with simultaneous pressure and heat treatment of samples during X-ray examination.

### EFFECT OF INTERACTIONS UPON DISPERSION OF NANOPARTICLES IN A POLYMER SOLUTION

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 polymer composites using larger filler particles. This new class of materials, nanocomposites, is a fast growing area of research with a wide range of applications in various fields, including optics, packaging, batteries, sensors, and others [1]. In this work, we study systems of nanoparticles and polymers through computer simulations. This method allows us to investigate the individual factors affecting the dispersion of nanoparticles in the polymer matrix. In particular, we examine the effects of nanoparticle–polymer interactions and relative volume fractions upon mean squared displacement, which can be linked to the degree of dispersion and agglomeration in the system.

#### Reference

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PUDDLE FORMATION IN LARGE DROPS MOVING THROUGH HIGH-VISCOSITY FLUIDS

Manohar Gottapu Chemical Engineering Faculty Research Advisors: Dr. Ileana C. Carpen and Dr. Pedro E. Arce

Mass transfer between droplets and a surrounding liquid is of central importance for many industrial processes such as extraction and the aeration of bioreactors. In the low Reynolds number regime (Re<<1), the buoyancydriven motion of a droplet accompanied by compositional gradients in a miscible high viscosity fluid is found to be different from the classical motion of the corresponding case of an immiscible droplet as given by the Hadamard-Rybczynski solution [2,3]. Previous and current experimental studies have shown that a 'puddle' region develops at the back/bottom of the drop due to convective-diffusive flows [1,4]. In this work, we examine a single spherical droplet in an infinite continuous phase. Herein we present a preliminary analysis that takes into account the partial miscibility of the drop with the ambient fluid, and qualitatively compare the predictions with experimental results.

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### ELECTROKINETIC ENHANCEMENT OF AIR SPARGING FOR GROUNDWATER AND SOIL REMEDIATION

Thorbjörn Holm (Royal Institute of Technology, Sweden; TTU) Chemical Engineering Faculty Research Advisors: Dr. Mario A. Oyanader and Dr. Pedro E. Arce

Air injection to soil for remediation purposes has been identified as a versatile application associated to various hydrocarbons clean up technologies, i.e. Air Sparging, Air Venting, Soil Vapor Extraction, Bio-venting, etc. An enhancement for the remediation technology has been proposed by adding an electrokinetic component to the hydrodynamic driving forces. A comparison between pressure profile predictions, along the depth of the capillary domain, is studied and numerically illustrated for the cases of several pressure differences, as well as including and excluding the electroosmotic force. The non-linear nature of the resulting transient of the differential model requires a rigorous numerical solution of the system of equations. Several details about model formulation, numerical solution, and behaviour of the model will be discussed in this contribution.

### KINETICS OF THERMAL DECOMPOSITION OF EXPANDED POLYSTYRENE (EPS)

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

The characteristics of thermal decomposition of expanded polystyrene (EPS) foams was studied in various gaseous environments, both oxidizing and non-oxidizing, over a narrow range of heating rates between 1 and 30 K/min using non-isothermal thermo gravimetric analysis (TGA). A modified integral-optimization technique was developed for multiple rate-controlling decomposition reactions, and results from kinetic data analysis shows that the activation energy of EPS foam decomposition in air is much less than any non-oxidizing environment, including nitrogen, helium and argon. Furthermore, qualitative mass spectrometric studies of EPS pyrolysis gases revealed the differences in EPS foam decomposition mechanism between various gaseous environments.

### MATHEMATICAL MODELING OF DISCHARGE BEHAVIOR OF CATHODE MATERIALS IN LI-ION BATTERIES

Uday S. Kasavajjula Chemical Engineering Faculty Research Advisors: Dr. Pedro E. Arce and Dr. Chunsheng Wang (now at U of Maryland)

Improving the rate capability of LiFePO<sub>4</sub> is a critical issue for commercialization of Li-ion batteries in hybrid electric vehicles and battery electric vehicles. In this study, the discharge kinetics of LiFePO, electrodes for Li-ion batteries were investigated by developing a novel mathematical model. The model is based on the theory of mixed mode phase transformation and it assumes that the phase transformation is controlled by both Li chemical diffusion and interface mobility. The discharge model was validated by comparing the model discharge curves with the experimental discharge curves of various LiFePO, samples from industry at different current densities. By using the validated model as a tool, effects of phase transformation, chemical diffusion, solid solution range, volume change and particle size on rate capability were determined and analyzed. The model developed here is applicable for any ion insertion electrode with a phase transformation (such as Li, Ti, O1, in Li-ion battery and metal-hydride electrodes in Ni/MH batteries).

### KINETICS OF CARBON VOLATILIZATION FROM FLY ASH

Narendar R. Mogulla and Jenny Bollig Chemical Engineering Faculty Research Advisor: Dr. Joseph J. Biernacki

The use of fly ash as a concrete admixture is dependent on the LOI (Loss on Ignition), which is primarily associated with free carbon content. American standards permit the use of fly ash with LOI < 6%. Carbon content in the fly ash mainly leads to inefficient performance of air-entraining admixtures, leading to increase in their dosage. Thus, it is essential to remove the carbon from fly ash to an acceptable level. Carbon burn out is dependent on the temperature and the availability of oxygen. The goal of this research is to explore the kinetics of carbon burn out from regional fly ash. The reaction order for carbon and oxygen, activation energy, and pre-exponential factor (constants) were determined from gravimetric data. The experiments were carried out non-isothermally with a constant heat rate and varying the oxygen levels to understand more thoroughly the kinetics and the role of oxygen in carbon burn out.

### BIOMEDICAL IMAGING GOLD NANOPARTICLES: TRANSFORMATION IN SURFACE WATER CONDITIONS

Vasanta L. Pallem Chemical Engineering Faculty Research Advisor: Dr. Holly A. Stretz Collaborator: Dr. Martha J. M. Wells (Center for Management, Utilization and Protection of Water Resources)

The aggregation behavior of gold nanoparticles in surface water was investigated. This particular class of nanoparticles represents significant commercial potential as novel platforms for drug delivery and biomedical imaging [1]; the fate and transformation of these particles post-use is of interest [2,3]. Environmental conditions such as pH, ionic strength, and humic acid composition were studied for their effect on aggregation behavior as detected by UV-vis spectroscopy [4]. The gold nanoparticles employed were synthesized and classified by transmission electron microscopy (TEM) [5]. Models for small angle neutron scattering (SANS) studies are also discussed.

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### ELECTROHYDRODYNAMIC VOLUMETRIC FLOWRATES FOR TRANSDERMAL DELIVERY OF CALCIUM-REGULATING HORMONES: EFFECT OF CAPILLARY GEOMETRY

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

Electrokinetic-based methods are used in a variety of applications including drug delivery and separation of biomolecules. Many of these applications use capillary bundle models to predict the behavior of the flow within the particular system. It is often assumed that within these bundles, capillaries of idealized geometries exist, including rectangular, cylindrical, and annular. Modeling flows in capillaries may be accomplished by applying the principles of electrokinetics in conjunction with hydrodynamics. In this project, capillaries of rectangular, cylindrical, and annular geometries are examined, for which velocity profiles are determined. Dimensionless functions for the volumetric flowrates for each geometry are determined from these velocity profiles, and a quantitative analysis is presented. Parameter values from the literature are used for the specific case for the delivery of calcium regulating hormones. Differences between the predictions by using the three geometries are studied parametrically and comparisons for possible minimal and large discrepancies are analyzed.

### ELECTROPHORESIS IN NANOPARTICLE-EMBEDDED POLYMER GELS: EFFECTS OF MORPHOLOGY

Jennifer Pascal Chemical Engineering Faculty Research Advisor: Dr. Pedro E. Arce, Collaborators: Dr. Mario A. Oyanader and Dr. Holly 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 to aid in the development of new pharamaceuticals, as well as tissue scaffold growth. The presence of nanoparticles within gels has the potential to modify not only the gel morphology but also the electrokinetic properties of the gels; therefore, these nanoparticles may influence both the electrokinetic transport inside the gels. This project focuses on capillary models whose characteristics are ideal domains to mimic the gel morphology. Such domains allow for the use of a nonuniform cross section and electrostatic potential along the capillary walls in order to capture the electrophoretic and electrostatic behaviors between the nanoparticles and the gel. This communication will report details and illustrations of the research performed.

### IDENTIFYING ADDITIONAL TOXIC COMPOUNDS PRESENT IN DRINKING WATER USING I-QSAR TECHNIQUE

Rushang B. Patel Chemical Engineering Faculty Research Advisor: Dr. Donald P. Visco, Jr.

In this work, we generate compounds that were not included in the contaminant candidate list (CCL) [1], which is published by the US- Environmental Protection Agency (US-EPA) periodically. The methodology involved is the inverse quantitative structure-activity relationship (I-QSAR) method using the molecular descriptor called signature. [2-3] The properties considered are the log D values at 7 pH, LD50 values for rat and mouse. We derive the height-1 (H-1) signatures for the training set that consists of 7 compounds recognized by the US-EPA. Then using the knowledge of the signature database and the descriptor matrix, we derive the constraint equations and solve them. We generated around 300 million solutions and after screening through various screens and regenerating those solutions [4], we ended up 258 compounds. We categorized those compounds into 36 different groups based on their structures for further studies.

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### REAL-SPACE (MILLI-SECONDS) SIMULATION, PARAMETER ESTIMATION, AND OPTIMIZATION OF LITHIUM-ION BATTERY MODELS

Robert Phillips, Dr. Vijayasekaran Boovaragavan, and Vinten D. Diwakar Chemical Engineering Faculty Research Advisor: Dr. Venkat Subramanian

Recent interest in lithium-ion batteries for electric and hybrid vehicles, satellite, defense and military applications has increased the demand on the computational efficiency of lithium-ion battery models. For analysis and control of lithium-ion batteries in hybrid environments (with a fuel cell, capacitor or electrical components), there is a need to simulate state of charge, state of health, etc. of Lithium-ion batteries in real-time. To optimize the hybrid environment, there has to be effective parameter estimation. Rigorous physics based models take up several minutes to simulate discharge curves depending on the solver, routines, etc. This poster presents an effective approach [4, 5] to simulate physics-based lithium-ion battery models in real-time (milliseconds) to facilitate control of electrochemical components in the hybrid environment by estimating vital parameters [6] (state of charge, state of health, etc.) and consequently making optimized process decisions [7].

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### CHARACTERIZATION OF VOLATILE ORGANIC COMPOUNDS (VOCs) IN COMMERCIAL KITCHEN EXHAUST EMISSIONS

### Rupesh K. Puttagunta

**Chemical Engineering** 

Faculty Research Advisor: Dr. Dennis B. George Collaborators: Dr. Pedro E. Arce and Dr. Martha J. M. Wells (Center for the Management, Utilization, and Protection of Water Resources) Commercial cooking operations are major source of particulate matter and volatile organic compound concentrations in urban areas. Particulate matter (<2.5 mm) emission rates reported from charbroiling of hamburger alone were as high as 40g /kg of meat cooked. In the present study, exhaust air emissions from commercial fast food appliances including gas fired char broiler (continuous and batch), electric clamshell, gas fired fry station and food products including hamburger, chicken fillet, fish fillet and French fries were monitored for volatile organic compounds (VOCs). The objective is to characterize and select dominant VOCs in the exhaust air emissions from commercial cooking operations and study their photochemical degradation kinetics. A modified EPA Method TO-17 protocol was used to sampling air through sorbent packing and collect VOCs. The samples were analyzed by a thermal desorption-capillary GC/MS analytical procedure. Results of this analysis and their implications for further research will be discussed.

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### EVALUATION AND COMPARISON OF LOCAL LIGHT INTENSITIES OF UVC LAMP FOR A PHOTO-REACTOR

Rupesh K. Puttagunta

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

Increased use of advanced oxidation processes (AOP) like photochemical processes to treat organic contaminants in water and exhaust air arise the interest to understand radiation profile of lamps used for photochemical reactions. Rates of photodegradation of contaminants are determined accurately when the radiation profile of the lamp inside the reactor is known. In the present study, local light intensities of a low-pressure mercury arc lamp producing UVc radiation are measured along the radius and longitudinal axis by chemical actinometry; these data are then compared with the values predicted from line source emission models. Simulated and experimental data are in good agreement with each other. The radiation field information will be used in kinetic studies of degradation of contaminants in the photo-reactor.

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NANOPARTICLE-COMPOSITE GELS FOR PROTEIN SEPARATION: SYNTHESIS AND PRELIMINARY CHARACTERIZATION

Hope E. Sedrick, Jennifer R. Bollig, and Nancy A. Burns Chemical Engineering Faculty Research Advisors: Dr. Holly A. Stretz and Dr. Pedro E. Arce

Nanocomposite gels offer great potential to modify the transport of proteins and DNA in purification and diagnostics protocols. We are currently using charged nanoparticles to template the internal gel architecture both structurally and in terms of electrostatics. In the current project, polyacrylamide gels were successfully cast as composites with charged nanoparticles of varying diameters (Southern Clay Laponite RD and an experimental Laponite). The dispersion of the nanoparticles, or filler, is characterized by the visual clarity of the resultant gels and acoustics. Preliminary electrophoresis runs comparing these novel architecture gels in electrophoretic separation efficiency will be presented. Future work includes modifying the gel morphology and the electrostatics characteristics of the nanoparticles to test their behavior in the above mentioned protocols.

### POLYACRYLAMIDE GEL MODIFIED WITH PNIPAM COATED GOLD NANOPARTICLES FOR ELECTROPHORESIS

Jyothirmai J. Simhadri Chemical Engineering Faculty Research Advisors: Dr. Holly A. Stretz and Dr. Pedro E. Arce

Traditionally, separation of proteins was accomplished by polyacrylamide gel electrophoresis; usually, gel structure is modified by change in concentrations of polymers in solution. Modifying structure of gels by either "macro-voids" (Rill et al, 1995) or by adding nanoparticles (Thompson et al, 2007) have proven successfully in increasing separation efficiency. Two classes of materials that have attracted a lot of attention are polymeric stimuli-responsive gels, such as poly-N-isopropylacrylamide (PNIPAm), and metal nanosize particles such as gold colloidal particles (AuNP). It is reported [Zhao et al, 2006] that AuNP's/PNIPAm hydrogel composites have thermo-switchable electrical properties. In this report, we propose a method for the synthesis of PNIPAm coated AuNP's and their dispersion into a polyacrylamide matrix; the resulting composite gels are hypothesized to enhance electrophoresis separations. Characterization of the material structure and electrophoresis on albumin proteins will be performed to confirm the effectiveness of the modified gel matrix on their separation efficiency.

### 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 the 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  $10^{-6} \mu m$ ) 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 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.

### ELECTROKINETIC-SOIL REMEDIATION: ROLE OF THE JOULE HEATING EFFECT ON ENGINEERING MODELS FOR THE TRANSPORT OF CONTAMINANTS

Cynthia Torres Chemical Engineering Faculty Research Advisors: Dr. Mario A. Oyanader and Dr. Pedro E. Arce

An engineering-type of mathematical model is here developed to understand the role of Joule heating on the mechanisms of migration during the electro-kinetic treatment process. One important aspect to be analyzed is the role played by buoyancy driving forces in the convective-diffusion and migration of contaminants in the soil matrix. This model will be focused on studying the transport of heavy metals within the soil. A simplification of the system is proposed in order to obtain an efficient and preliminary analysis of the behavior of the system. The case of convective-dominated transport regime (i.e., Peclet àlarge values) is considered. This important case is handled with a solution based on the methods of characteristics proposed by Acrivos and collaborators. In the poster presentation several aspects related to the assumptions used, simplifications made and solution methodology will be summarized. Observations of the system behavior and future efforts will be also offered.

### VIRTUAL SCREENING PubChem FOR FACTOR XIa INHIBITORS USING SIGNATURE

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

In early stages of drug discovery high-throughput screening (HTS) is often utilized to uncover new lead compounds. In this process, robotic machines are used to rapidly test large libraries of compounds for a specified target. Results from HTS funded by the National Institutes of Health (NIH) are deposited for the public via the PubChem database. [1] Bioassay 846 screened for novel anticoagulant therapeutics by identifying inhibitors of the enzyme factor XIa, which is involved in the blood coagulation mechanism. [2] In this work, we utilize the data collected from bioassay 846 to develop a quantitative structure-activity relationship (QSAR) and virtually screen ~12 million compounds also deposited in PubChem. QSARs are models which apply descriptors to relate the structure of a compound to a specific molecular property of interest. The molecular descriptor used here encodes all atoms a pre-defined height h away from the root atom, and is known as Signature. [3] Compounds identified as active from the virtual screen form a focused database suitable for further study.

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### AUTOGENOUS STRAIN IN HYDRATING PORTLAND CEMENT

Albert A. Wilson and Sean E. Mikel Chemical Engineering Faculty Research Advisor: Dr. Joseph J. Biernacki

Development of autogenous strain in hydrating portland cement samples was investigated. Early-age shrinkage of hydrating cement is induced by several factors including capillary stresses that develop within the hardening cement matrix [1]. The progressive generation of the cement hydration product, CaOH, was measured over a period of time using X-ray diffraction. The X-ray spectra obtained were deconvoluted by fitting them to a combined Gaussian-Lorentzian function. The resolved spectra were used to calculate the d-spacing between CaOH centers. Changes in the d-spacing as a function of hydration time were used to estimate the development of strain induced within the hydrating cement matrix by the hydration process. The estimated strain using this method will be compared with data obtained by other empirical methods reported in the literature.

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### THE EFFECT OF FINE INERT PARTICLES ON PORTLAND CEMENT HYDRATION KINETICS

Tiantian Xie Chemical Engineering Faculty Research Advisor: Dr. Joseph J. Biernacki

The chemical reactions that occur during the early stages of portland cement hydration are complicated and the basic mechanisms yet debated. Furthering the complexity, modern cement systems incorporate fine admixtures such as slag, fly ash and silica fume. These also actively participate in the reaction process. To study the early stage hydration kinetics and the effect of additive particles, model systems containing inert particles (silicon carbide) were used. Samples containing particles in the amount of 30% inert material and 70% portland cement with a 0.35 water-to-cementitious ratio were investigated. The resulting specific heat of hydration was determined using isothermal calorimetry. Surprisingly fine "inert particles" accelerate the early stage hydration likely by providing surface areas for the nucleation and growth of products.

### MODELING AND EXPERIMENTATION OF POLYOL + BLOWING AGENT SYSTEMS

Satya Suresh Yelisetty Chemical Engineering Faculty Research Advisor: Dr. Donald P. Visco, Jr.

Polyurethane foams are made by reacting a di-isocyanate molecule with a polyol in the presence of a blowing agent. Solubility of blowing agent in the polyol plays an important role in determining the dimensional stability and quality of the polyurethane foam. Recently, concerns have been raised on high Ozone Depleting Potential of traditionally used blowing agents like chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs). Hydrofluoro-carbons (HFCs) have been identified to be long-term replacement as the future blowing agents. In this study, we measured the solubility of five zero ODP HFC's namelyHFC-125 (1,1,1,2,2-Pentafluoroethane), HFC-152a (1,1-Difluoroethane), HFC-143a (1,1,1-Trifluoroethane), HFC-32 (Difluoromethane), and HFC-245fa (1,1,1,3,3-Pentafluoropropane) in three polyols namely Pluracol 975, Pluracol 355, and Terol 352 using a degassed vapor pressure apparatus. The experimental data is correlated with SAFT-VR and Sanchez-Lacombe EOS.

### CHEMICAL ENGINEERING UNDERGRADUATE STUDENTS

COMPARISON OF METHODS TO DETERMINE PHASE EQUILIBRIA FROM EQUATIONS OF STATE

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

There are many practical uses for developing a dimensionless integration technique for single and multicomponent phase equilibrium calculations. Through the use of higher order numerical integration techniques, phase equilibrium calculations can be solved for pure component substances and mixtures. Utilization of these methods will hopefully lead to faster and more reliable calculation methods for determining phase equilibrium conditions via integration.

### MICROMIXING IN CAPILLARY CHANNELS WITH BUOYANCY FLOWS AND REACTION AT THE WALLS. EFFECT OF ASYMMETRIC CONDITIONS

Katherine Cerda Chemical Engineering Faculty Research Advisors: Dr. Mario Oyanader and Dr. Pedro E. Arce

In general, the effect of buoyancy driven flows on the hydrodynamics of a system is neglected to simplified or to isolate the influence of others driving forces. As it is well known, the hydrodynamics of a system can considerably change the dispersion of solute inside a capillary channel. When buoyancy is the primary hydrodynamic phenomena, neglecting its effect on velocity profile may not be such a good idea, considering the mixing effect that takes place. The authors have used the spatial averaging method in combination with the solute species continuity equation to determine the effect of buoyancy driven type flows on effective parameters, i.e., effective dispersion coefficient and effective convective velocity. This contribution includes a reacting phenomena at the walls. In this effort, explicit analytical expressions have been derived for the effective parameters as a function of the ambient temperature, skew temperature parameter and net mass flow. These mathematical expressions may be useful on the study of post-electrophoretic processes, such as electro-assisted drug delivery, micro-electrophoretic separations, soil remediation, and material processing where the temperature development are still present after electrostatic forces have been shut down. Several illustrations are presented to demonstrate the macromixing effect caused by buoyancy in a capillary channel of rectangular geometry.

### GENERATING SELECTIVE SEROTONIN REUPTAKE INHIBITORS (SSRI) USING THE QSAR ALGORITHM WITH SIGNATURE

Chris Heckman Chemical Engineering Faculty Research Advisor: Dr. Donald P. Visco Jr.

SSRIs are a class of antidepressants that work by raising the level of serotonin outside of the cell. A SSRIs quality can be judged by activity, half-life, number of side effects, and ease of synthesis. The goal of this research is to generate novel SSRIs, via I-QSAR, with a lower half-life and higher active in the body. An assay of 21 compounds was used to create 214 constraint equations. After solving these equations 8,939,088 solutions were generated. Current work includes, running the generated solutions through filters leaving only the solutions with high activity and a low half-life. After

filtering, the structures will be generated and filtered based on whether compounds are energetically favorable and if these compounds can even be synthesized. Further research will be done to confirm that the predicted properties are exhibited in vivo.

### NOVEL CORTICOSTEROID DEVELOPMENT VIA I-QSAR WITH SIGNATURE

Joshua D. Jackson Chemical Engineering Faculty Research Advisor: Dr. Donald P. Visco

The research discussed here involves the development of a class of preventative asthma medications named corticosteroids. Corticosteroids such as hydrocortisone have commonly been the therapy of choice where an antiinflammatory or immunosuppressive treatment is required. The focus of this research is to develop novel corticosteroids that are highly selective toward the lungs and are promptly removed from the body when exposed to the main circulation. We look to use the Inverse-Quantitative Structure-Activity Relationship (I-QSAR) algorithm with Signature to generate new drugs based upon the structures and corresponding activities of previously studied corticosteroids. I-QSAR explores possible combinations of atom connectivity, and structural filters are used to predict and collect the best candidates for further study. Our work currently focuses upon filtering the solutions generated from the inverse problem, leaving a database possessing only characteristics such as high receptor binding affinity, high systemic clearance, high plasma protein binding, and low oral bioavailability.

### AXIAL MICROMIXING IN CAPILLARY CHANNELS WITH ELECTROOSMOTIC FLOWS

Karina Merino

Chemical Engineering Faculty Research Advisors: Dr. Mario Oyanader and Dr. Pedro E. Arce

Soil clean up applications by electrokinetic process have demonstrated to be suitable for heavy metal removal in sites of difficult access as an in situ technique. The effect of different driving parameters has been identified and reported in the literature as an effort to unveil the optimal conditions of removal. Among others, pH profile variations along the treatment zone have been linked as an important parameter to process efficiency. Studies have indicated that under certain condition axial flow reversals occurs affecting contaminant removal. Validating this assumption is important as well as identifying the implicated results. In this study a particulate movement is simulated for different case scenarios. The primary mechanisms considered in the approach are electroosmosis and drag forces. The theoretical analysis has been closely monitored and compared with laboratory results. Meaningful illustrative results are presented along with the most relevant conclusions. The idea behind the study is to explain the experimental results via theoretical modeling and simulation.

### PUDDLE FORMATION IN MOVING DROPS AT LOW REYNOLDS

Adrian Mether Chemical Engineering Faculty Research Advisors: Dr. Ileana Carpen and Dr. Pedro E. Arce

In the earth's mantle, sections of hot magma rise through cooler, denser layers, in the process entraining some of the surrounding fluid and forming structures known as diapirs. The process is affected by gradients in temperature and viscosity, as well as chemical composition, possibly. This research focuses on providing a better understanding of this phenomenon. To do so, we consider a simple experimental model of a fluid drop moving through a second, partially miscible fluid. With the temperature kept constant, fluid motion will mainly be affected by mass transfer. Buoyancy (due to density differences between the two fluids) causes the drop to rise (or fall), while mass transfer will induce changes within the drop and fluid properties over time, with a corresponding effect on the flow profile. The analytical solution to the limiting case of immiscible fluids is studied as preliminary background.

### DESIGNING EFFECTIVE TRIALS REGARDING TREATMENTS AGAINST CANCEROUS TUMOR GROWTH

Nemoy Rau Chemical Engineering Faculty Research Advisor: Dr. Ileana Carpen

Cellular adaptation to changing environments is intricately coordinated through many molecular and mechanical responses. As cells evolve, abnormal growth patterns occur (that cannot be controlled by normal mechanisms) leading to cancer. With mathematical modeling we can integrate different characteristics of tumor growth for a nonexperimental study of cancer. [1] Through integration of some of the prior clinical, experimental, and mathematical studies, we utilize a cellular automata model to take into account multiple factors affecting tumor growth in healthy tissue. [2] This in silico simulation model of tumor growth is based upon molecular and life cycle features that effect the growth rates of cancer. The life cycle parameters used in this model include replication rate, nutrient concentrations for proliferation and survival, and possible drug effects. [3] This

3-D in silico model is used to study the effects of drugs upon the growth and development of the tumor and optimize a drug treatment protocol under various conditions.

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TWO PHASE LIQUID FLOW IN A CAPILLARY REACTOR

Philip Schmitt, Heather DeBord, and Johnathan Wheeler Chemical Engineering Faculty Research Advisors: Dr. Holly Stretz and Dr. Pedro E. Arce

The two-phase reactor is intended to optimize the surface area for reaction contact versus the separation of two phases downstream without coalescers. Minimizing cost of separations is important because they are expensive. The two phase reactor will make the separations less expensive. An example of phase transfer catalyzed two-phase reactions is the production of Bio-diesel. A two-phase, continuous flow reactor was constructed with an organic phase high-flow pump and an aqueous phase low-flow pump. The objective is to calibrate the flows on both pumps using a Newtonian fluid and obtain data for pressure drop versus volumetric flow rate to be used in forming a modeling. It is expected that the distance between the fibers is either nanoscale or capillary scale, neither which can be measured visually. The data will be used to identify the scale for the distance between the fibers. The long range goal is to produce a fluid dynamics simulation of flow characteristics versus postreactor separation.

ZETA POTENTIAL OF POLY(N-ISOPROPYLACRYLAMIDE) STABILIZED GOLD NANOPARTICLES; FLUORESCENT TAGGING OF GOLD NANOPARTICLES FOR MICROSCOPY. A PROPOSAL FOR UNDERGRADUATE RESEARCH

Melissa Taylor, Vasanta Pallem, and Jyothirmai Simhadri Chemical Engineering Research Advisors: Dr. Holly Stretz and Dr. Pedro E. Arce Gold nano-particles can be appropriately tagged to fluoresce for microscopy. Gold nanoparticles will be monodispersed and coated with poly (N-isopropylacrylamide) and then fluorescently tagged. These particles should then be able to be able to fluoresce on available instruments of the engineering department. These nano- particles will then be characterized by ultraviolet visual microscopy. The results of this proposed research will be accumulated to indicate paths traveled by the tagged gold nano-particles. The results are important to understand the behavior of nanoparticlcles in materials such as composite gels for electrophoresis.

ZETA POTENTIAL: ANALYSIS AND MEASUREMENT IN NANO-PARTICLES. A PROPOSAL FOR UNDERGRADUATE RESEARCH

Melissa Taylor Chemical Engineering Faculty Research Advisors: Dr. Pedro E. 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 nano-particle will be studied and possibly measured. Model equations that examine the relationship of zeta potential versus the charge in nano-particles will be developed. Furthermore, experimental techniques suitable for the measurement of zeta potentials will be identified and related to the model equations. By implementing experiments using both equations and proper instruments, zeta potentials will be acquired to make accurate predictions of surface charged of the nano-particles and their variances with different conditions.

### THERMALLY RESPONSIVE MICROPARTICLE GEL ELECTROPHORESIS

Jeff Thompson Chemical Engineering Faculty Research Advisors: Dr. Holly Stretz and Dr. Pedro E. 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(Nisopropyl 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. Both UV and visual characterization are used to determine and compare the transport (i.e. mobility and dispersion) characteristics of the new gels with standard gels in the electrophoresis runs. A composite of one percent by mass PNIPAM and four percent acrylamide offers separations which are not available for five percent acrylamide concentration using albumin markers.

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### CIVIL AND ENVIRONMENTAL ENGINEERING GRADUATE STUDENTS

MODELING THE HYDROLOGICALLY-RELEVANT FEATURES OF UNCERTAINTY OF NASA'S HIGH RESOLUTION PRECIPITATION PRODUCTS FOR ADVANCING GLOBAL APPLICATIONS OVER UNGAUGED REGIONS

Ling Tang

Civil and Environmental Engineering Faculty Research Advisor: Dr. Faisal Hossain

In the post 2013 era of the NASA's Global Precipitation Measurement (GPM) mission, high resolution precipitation products (HRPP) from satellites will become increasingly common for various global hydrologic applications overland (such as flood detection using distributed models). For advancing the application of these datasets, the associated uncertainty information will therefore be critical for users to understand the realistic limits to which these HRPPs can be applied over an ungauged region. However, this represents a paradox. Satellite rainfall uncertainty estimation requires ground validation (GV) precipitation data. On the other hand, satellite data will be most useful over ungauged regions in the developing world that are lacking in GV data. The primary objective of this proposal is therefore to reconcile this paradox with the motivation to further unleash the potential of NASA's HRPPs for the developing world. Two important science questions are hoped to be answered through this project as follows. 1. How much climatologic classification of error regime is possible for characterizing uncertainty of NASA's HRPPs? 2. If "error" is defined on the basis of ground validation (GV) data, then how can uncertainty be estimated for NASA's global rainfall data products without the need for extensive GV data?

### LARGE DEFORMATION ANALYSIS OF RECTANGULAR PLATES USING THE GROEBNER BASIS

Robert Wade VanDervort III Civil and Environmental Engineering Faculty Research Advisor: Dr. Y. Jane Liu

In modern structures a high strength to weight ratio is one of the desired properties for materials. Engineers can now design lighter structures with stronger materials, but this also requires change in the way they analyze these structures. For example, when the displacement of a plate is large when compared to the thickness, the assumptions in the classical analysis of the plate are no longer accurate. Therefore, geometrically non-linear provisions must be made to accurately model the large deformation behavior. The objective of this research is to apply the computational method of Groebner basis to the non-linear analysis of plates. The Groebner basis is an efficient tool from algebraic geometry that can be used to solve a system of non-linear algebraic equations by expressing them in an easier algebraic system of which exact solutions can be determined. The results demonstrate that this computational method has promising potential in engineering applications.

### CIVIL AND ENVIRONMENTAL ENGINEERING UNDERGRADUATE STUDENTS

A REVIEW OF THE STATE OF THE ART OF TREATIES IN RELATION TO MANAGEMENT OF TRANSBOUNDARY FLOODING IN INTERNATIONAL RIVER BASINS

Caitlin B. Balthrop Civil and Environmental Engineering Faculty Research Advisor: Dr. Faisal Hossain

The destruction caused by floods worldwide becomes worse when there is lack of adequate preparation in advance. In particular, the flood-prone international river basins (IRBs), i.e., basins that are made up of many different countries, nations that are located close to a basin's outlet face a major problem in effectively monitoring floods. However, a planned international satellite mission that has positive implications on the monitoring of transboundary flooding is the Global Precipitation Measurement (GPM) mission. GPM is scheduled for launch in 2013. In order to provide coherent evidence to the legislative community, that GPM can indeed be a globally beneficial mission, the state of the art on water treaties in relation to transboundary flooding in

IRBs was reviewed. The Transboundary Freshwater Disputes Database maintained by Oregon State University was the primary source of information. Twenty-five treaties were identified that had some allusion to dealing with flood control and water allocation to downstream nations. The review highlighted a few basins that have recurring flooding issues. It also showed basins that are multi-nationally monitored. However, the review clearly verified that existing treaties do not have any mechanism for riparian nations to share real-time rainfall information during an impending transboundary flood event. The review offered insight to pathways of future research and verified that GPM, when launched, has the potential to alleviate the current problems on transboundary flood management that are made worse due to an absence of proper water treaties among nations.

### EXPANSION OF CEMENTITIOUS MORTARS DUE TO DELAYED ETTRINGITE FORMATION

Lindsay Smith Civil and Environmental Engineering Faculty Research Advisor: Dr. Benjamin Mohr

This research is aimed at investigating the mechanisms of delayed ettringite formation causing expansion in portland cement mortars. The formation of ettringite is a normally benign product of cement hydration that occurs at early ages. However, ettringite is increasingly observed in concretes that have been in service for many years. Often associated with the ettringite observation is cracking of concrete. 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.

### ELECTRICAL AND COMPUTER ENGINEERING GRADUATE STUDENTS

AN EFFICIENT EMBEDDED SYSTEM DESIGN FOR CAPTURING AND STORING ANALOG DATA

Mohammed Abdallah Electrical and Computer Engineering Faculty Research Advisor: Dr. Omar Elkeelany and Dr. Ali Alouani Existing microprocessor-based data acquisition systems are cumbersome, expensive, and have limited mobility. Part of the problem is the lack of integration of different components of such systems. Recent advances in systems-on-a-chip technology allows for compactness and integration. Micro processor based data analysis and interpretation requires acquired data in a digital format. To design future handheld data acquisition system, one needs to capture signals and store them into a non-volatile digital memory device. When writing to a Flash memory, existing systems require a micro processor. A prerequisite to the design of future handheld data acquisition system is the development of a Flash memory controller that writes data directly to a Flash memory device, without using a micro processor. The aim of this paper is to design an efficient Flash memory controller that writes temporary collected data to a detachable Flash device. To achieve this task without the need of a micro processor, systemson-a-chip design technology will be used. We analyze two mechanisms, to store these signals into a secured digital card. The first approach uses single-block write and the second one is based on the multiple-block write. This paper shows that the multiple-block write mechanism is more efficient in terms of the time it takes to store the temporary acquired signals into the secure digital card.

### DISTRIBUTED GENERATION PLACEMENT DESIGN IN MATLAB DISTRIBUTED COMPUTING

Xi Chen

Electrical and Computer Engineering Faculty Research Advisor: Dr. Wenzhong Gao

Distributed Generation (DG) is a promising solution to many power system problems such as voltage regulation, power loss, etc. The location in the power system for DG placement is found to be very important. The additional DG placement strategy is also found to depend largely on the total capacity and location of DG already installed on the system. In this study, a design strategy based on a proposed "critical bus tracking" method for Proton Exchange Membrane Fuel Cell (PEMFC) DG is tested on a modified IEEE 14 bus test case [1]. Matlab Distributed Computing System (MDCS) [2] is applied for a reduced computation time. Program for contingency analysis [3] [4] is also implemented in MDCS to test the design strategy. Tests are conducted in the modified IEEE 14 bus and 300 bus test cases to study the efficiency of the parallel algorithm for DG placement design and contingency analysis.

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### AN ONLINE CONTROLLER TOWARDS FILE SYSTEM AVAILABILITY AND PERFORMANCE

#### Xin Chen

Electrical and Computer Engineering Faculty Research Advisor: Dr. Xubin He

Nowadays, one challenge when building a large-scale distributed file system is maintaining both high availability and high performance [1]. Although many fault tolerance technologies have been proposed and used in both commercial and academic distributed file systems to achieve high availability, a tradeoff between availability and performance always exists for any fault tolerance. For example, to achieve higher availability, RAID may scarify performance by increasing reconstruction speed [2], and replication technology may increase the number of creating replica actions which may occupy more I/O and network resources [3, 4]. In this paper, we analyze the tradeoff between file system availability and performance, and this analysis leads to a design of controller that will make system satisfy the minimal requirements of file system performance and availability for a running application.

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### IMPROVING SPATIAL MAPPING OF ARSENIC CONTAMINATION IN GROUND WATER TO PREVENT HEALTH HAZARD

### Mohammad Chowdhury

Electrical and Computer Engineering Faculty Research Advisors: Dr. Faisal Hossain (Civil and Environmental Engineering) and Dr. Ali T. Alouani (Electrical and Computer Engineering)

Dissolved arsenic in groundwater poses health risks in many part of the world. Because of the expensive and timeconsuming nature of arsenic concentration measurement, it is not possible to continuously sample the groundwater extensively in a given country. Developing countries with limited resources particularly suffer from the lack of a continuous monitoring system. It is therefore desirable to estimate the arsenic concentration across the country using the limited number of measurements available and attempt to extract the maximum amount of information on the spatial and temporal patterns. The commonly used technique for this purpose is the kriging technique. Such a technique uses linear interpolation that does not account for the spatially nonlinear and chaotic behavior of arsenic contamination. The purpose of this study is to use learning systems (such as Artificial Neural Networks) to provide more accurate spatial estimate of the arsenic concentration using the same limited amount of measurements. Contrary to existing approaches, the learning system based approach makes no assumption about the nature of the propagation of contamination in ground water. The approach takes advantage of the leaning and generalization ability of artificial neural networks to perform a more accurate estimation.

### MEASUREMENT OF TOWER FOOTING RESISTANCE USING MAGNETIC FIELD SENSORS

Aneesh A. Davalbhakta Electrical and Computer Engineering Faculty Research Advisor: Dr. Satish M. Mahajan

Low footing resistance of a transmission pole is desired as it affects switching surge performance and surges caused by lightning strikes to power transmission lines in the distribution system. This footing resistance must be

measured periodically. It changes with change in weather, soil type. A method called "Single Point System" was used to measure the footing resistance of a transmission pole using magnetic field sensors even with ground wire attached [1-3]. This work represents different ways of mounting Giant Magnetoresistive (GMR) sensors on a pole. A method called "Single Sensor System" based on Single Point System is described. Application of Single Point System as to measure resistance of a grounding grid is also discussed. Currents in the range of 1mA to 3mA were used. Error in the measurement of a tower footing resistance and model of a grounding grid resistance was observed to be within 5% [4].

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### ELECTRICAL CAPACITIVE TOMOGRAPHY SENSOR FOR ESTIMATING METAL FILL PROFILE IN LOST FOAM CASTING

Wael A. Deabes

Electrical and Computer Engineering Faculty Research Advisor: Dr. Mohamed A. Abdelrahman

Lost foam casting (LFC) process is one of the most energy efficient casting methods in the industry [1]. The metalfill profile (MFP) is one of the important factors that affect casting quality. Monitoring the fill profile is one the important indicators of problems in the casting process [2, 3]. Hence the characterization and the control, if possible, of the metal fill are essential in LFC. Electrical capacitive tomography (ECT) sensors [4], based on measuring the change in the coupling capacitance in the presence of grounded metal in its proximity, provide a simple nonintrusive visualization technique of acquiring the metal profile [5]. Rugged and noninvasive array of capacitive electrodes are mounted around a target area. These measure the inter-electrode capacitance changes caused by variations of the grounded metal inside the target area. These electrodes can be used to identify fill time during the casting. However, deducing the metal fill distribution from the measurements is a difficult problem. This poster reports developments towards an algorithm for determining the fill profile. The system is intended for use on the foundry floor, thus the designed system has been made wireless, non-intrusive and a limited number of measurements are used to lower cost of hardware. An iterative linear back projection (ILBP) [6, 7] technique for solving the MFP problem is adapted. The proposed method is able to detect the position of the metal in a simulated environment using only 6 measurements from the sensors. Results from experiments carried out on different metal locations using the proposed technique are reported.

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### INDEX-BASED REACTIVE POWER COMPENSATION SCHEME

Damian O. Dike Electrical and Computer Engineering Faculty Research Advisor: Dr. Satish M. Mahajan

Since the large scale introduction of Flexible AC Transmission System (FACTS) devices to support the distressed power grid without robust index to measure their impact on interconnected power system in the nineties, there has been increase in the number of notable power system

outages [1-4]. This development has opened up interest in the need for efficient reactive power utilization in the grid [5]. To improved the application of FACTS and contribute to the mitigation of power outages associated with current near-limit operated commercialized grid, this research work is focusing on the development of a voltage stability indexbased reactive power compensation scheme. Considering current regional wheeling of power, a new complex power  $\pi$  – structure index model suitable long transmission lines will be incorporated into multi-FACTS Newton-Raphson's load flow [6] & [7]. This model will be simulated using IEEE 14 and 30 bus systems with FACTS and microgrid separately interconnected under varying conditions.

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### BATTERY CHARGING CONTROL TECHNIQUE FOR HYBRID ELECTRIC VEHICLE

Sharanya Jaganathan Electrical and Computer Engineering Faculty Research Advisor: Dr. Wenzhong Gao

Environmental protection place restrictions on the emission of waste gases from the motor vehicle and motorcycle thus accelerating the development of electric vehicles and hybrid electric vehicles driven by electricity. At present there are a lot of technical problems for the batteries of EV and HEV such as life cycle of battery, convenience of charging, fast charging, promotion of energy density, performance and low cost. The objective here is to develop a novel control strategy and a low cost high performance power electronic device for charging the battery. The work will also include comparing different charging methods to study their effects on the overall energy efficiency. The charging technique will be implemented in Simulink/Matlab or equivalent software. Also the simulation results will be validated with the experimental set up to check the effectiveness of the technique.

### DATA DISSEMINATION METHODS IN WIRELESS SENSOR NETWORKS

Manjeera Jeedigunta Electrical and Computer Engineering Faculty Research Advisor: Dr. Xubin He

Wireless Sensor Networks is a field that is growing in importance with every passing day [1]. With applications ranging from military [2] to simple habitat monitoring [3], sensor networks offer a vast potential for research. The cumulative amount of data generated by these networks with a large number of nodes would be high, as a result of which Data Storage Techniques are highly important [4]. This research aims at investigating the various techniques of data dissemination. We present the underlying structure that most data dissemination algorithms in sensor networks follow and analyze the performance metrics significant in evaluating a data dissemination algorithm.

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### FULL ORDER MODEL ANALYSIS OF A FIVE PHASE INDUCTION MACHINE

Sosthenes F. Karugaba Electrical and Computer Engineering Faculty Research Advisor: Dr. Joseph O. Ojo

The induction machine is the most used in all practical applications requiring variable speed due to its robustness, versatility and reliability. Induction machines having threephase windings are normally used, since standard power supply is three-phase. However, when fed by an inverter, there is no need for fixed number of phases, some other phases being possible and advantageous. Drives with more than three phases have various advantages over conventional three-phase drives, such as reduction in amplitude and increase in frequency of pulsating torque, reduction in harmonic currents [1, 2]. Five-phase machines can develop torque using both fundamental and higher harmonics of air gap field [3]. Hence the analysis, design, and application of such machines require adequate mathematical models to be established through which their performance and advantages can be evaluated. In this work, therefore, the analysis of a full order model of a five-phase induction machine is presented.

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### MODELING AND CONTROL OF A COUNTER-GRAVITY CASTING MACHINE

Ameer M. Khader and Wael A. Deabes Electrical and Computer Engineering Faculty Research Advisors: Dr. Mohamed A. Abdelrahman and Dr. Charles Carnal

Counter-gravity casting is a process where molten metal is forced into the casting cavity against gravity. It aims at increasing the energy efficiency of the casting process. It also offers an opportunity of introducing automatic control into the process by changing the pressure under which the metal is forced into the mold cavity [1, 2]. This work describes a new method of multi-variable control of the counter-gravity casting machine. System modeling of the counter-gravity machine reveals that it is a nonlinear system [3-5]. The machine has been modeled as a set of linear systems corresponding to twelve regions of operation: six for increasing vacuum and six for decreasing vacuum. The models are parameterized based on the stem valve positions and the initial pressure in the casting vessel. The models are validated through actual data collected from the countergravity machine. An automatic controller is designed for control of the machine operation throughout the different regions. The full scheme of the controlled simulated machine consists of a valve selector and a gain scheduled controller based on the operating conditions of the machine. Simulations are provided to show the operation of the designed controller.

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### SAG MONITORING USING GLOBAL POSITIONING SYSTEM

Shalini Sushmitha Komaragiri Electrical and Computer Engineering Faculty Research Advisor: Dr. Satish Mahajan

A new method to measure the physical sag of an overhead conductor line involves differential global positioning technique [1], [3]. The method relies on the information received from the GPS satellites and is capable of measuring sag to an accuracy of approximately 2 cm using a commercially available LEICA GPS System [2]. However, the overall cost of the system (~ \$50 K) is somewhat high [2]. Proposed method of using three or more cheaper GARMIN GPS devices to measure sag, could be a cost effective

alternative to the expensive LEICA GPS System. The GARMIN GPS devices when placed on the same horizontal plane gave an accuracy of about ±8 meters with reference to LEICA GPS System. Therefore, various factors affecting the accuracy of cheaper GARMIN GPS devices and various mathematical algorithms for error correction are being investigated in this research.

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### ENHANCED VERDET CONSTANT VIA QUANTUM DOT DOPED GLASS SAMPLES

Ganapathy Kumar

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The Faraday Effect or rotation of plane polarized light in glass samples under the influence of an external magnetic field and the Faraday rotation angles is reported for SF-57, BK-7 and borosilicate type glasses. Doping the glass with quantum dots increases the electron confinement energies upon excitement and magnifies the phase difference between the right and left circularly polarized light thus enhancing the Faraday rotation angle and hence the Verdet constant for that material, which is dependent on wavelength and temperature, resulting in high magnetooptic effect. The measured Verdet constant values were 11.25 deg/T-cm, 2.67 deg/T-cm and 0.1295 deg/T-cm for undoped SF-57, BK-7 and borosilicate rods respectively and conform to literature [1-4]. The application of these types of glasses can be done to Magneto-Optic Current transformers (MOCTs), Optic fiber current sensors and highly sensitive current detectors [5, 6].

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### ANTI-ISLANDING DETECTION ALGORITHM FOR DISTRIBUTED GENERATION

### Rohit Kunte

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In recent years there have been changes in the distribution system configuration due to inclusion of DGs at the distribution level [1]. DG sources contribute in improving the power quality, minimizing peak loads and reducing the need for reserve margin. Distribution systems have been traditionally designed as radial systems, and time coordination of protective devices has been a standard practice used by the utilities. But the insertion of DGs to these radial systems requires change in protection strategy. Islanding in power systems refers to the condition where a portion of the grid is solely supplied by the DGs and that this part is isolated from the rest of the power system [2]. This condition presents potential hazards to the utility personnel as well as the consumers. Our objective is to develop a new anti-islanding detection algorithm that can effectively detect islanding in power systems. Matlab-Simulink software has been is used to simulate and test the algorithm. The work has been done with wind generator as a DG source. Though the method gives excellent results it is applicable to limited scenarios. The current work concentrates in widening the scope of this method with the help of feedback technique. Also there is a plan to test the new algorithm experimentally with wind turbine and PV source acting as DG sources along with the utility.

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### DISK DRIVE FAILURE FACTORS

Jeremy Langston Electrical and Computer Engineering Faculty Research Advisor: Dr. Xubin He

Reliability has emerged as a major player in the evergrowing demand for data storage, particularly in medium to high-end computing systems such as those found at Google and Yahoo! [1]. A primary concern in overall storage reliability is that of hard disks, where the data is ultimately stored [2]. Modern disk drives have become highly complex with increasing demands on high throughput, high reliability, high capacity, and low cost - which are typically mutually exclusive. This research delves into the factors that cause a drive to fail, thus impacting storage system reliability. Failures fall into three main categories: hardware, software, and process. Frequent factors are given, focusing on data thrashing, disk age, and hot spots [3–5].

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### DATA PLANE PERFORMANCE ANALYSIS IN HETEROGENEOUS NETWORKS

#### Dina Machuve

Electrical and Computer Engineering Faculty Research Advisor: Dr. Stephen Parke Collaborators: Dr. Nasir Ghani and Qing Liu (University of New Mexico)

Detailed performance evaluation of the data plane technologies have focused solely on homogeneous technology domains e.g. delay/loss performance in QoS packet-switch networks, jitter in SONET/DWDM networks. Future end-user applications will be run over many heterogeneous networking layers (i.e. both packet and circuit switching) with requirements for high and stable bandwidths. The United States Department of Energy (DOE) runs a full national IP/MPLS backbone, the Energy Sciences Net (ESNet) [1], a live production network offering "carrier-grade" support. DOE is also experimenting with and advanced optical DWDM backbone, the Ultra Science Net (USNet) [2] to achieve high-end gigabit throughput. The data plane models developed for network simulation include MPLS routers, Ethernet switches, SONET/SDH and optical DWDM. The main goal of performing network simulation is to verify and corroborate empirical findings in network simulation environments [3]. The performance metrics used are delay, jitter and throughput.

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### DESIGN OPTIMIZATION OF A 35nm INDEPENDENTLY-DOUBLE-GATED FLEXFET SOI TRANSISTOR

Rama Satyanarayana Chintala, Himaja Reddy Moolamalla, Ken Modzelewski, and Nishanth Gudipelly Electrical and Computer Engineering Faculty Research Advisor: Dr. Stephen A. Parke

Planar independently-double-gated Flexfet CMOS transistors have been developed, which exhibit strong

dynamic threshold voltage control of 0.3-1.0 V\V. The Flexfet device incorporates a mid-gap MOSFET top gate self-aligned to an implanted silicon JFET bottom gate. Each transistor in a circuit may be connected in either single-gate (SG), double-gate (DG), or independent-double-gate (IDG) mode as needed to achieve ultra-low-power CMOS ICs. A simple analytical dynamic threshold voltage model was developed and verified by using SILVACO ATLAS device simulation software. Design optimization of a 35nm independentlydouble-gated Flexfet Silicon-On-Insulator transistor with an ideal 1.0V\V dynamic threshold control of this device was achieved. The device used for simulation and the analytical threshold model developed are in 2D but a 3D complex model will also be developed. Since the threshold voltage of the device varies due to short channel effects at 35nm, optimization was done to overcome these effects.

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### APPLICATION OF GENETIC ALGORITHM IN ELECTRIC DISTRIBUTION SYSTEMS

Ndaga Mwakabuta Electrical and Computer Engineering Faculty Research Advisor: Dr. Arun Sekar

To achieve optimal operation of distribution systems, some optimization techniques must be applied. The distribution system models contain functions that are not easily solved by conventional algorithms. Evolutionary optimization algorithms provide solution that handles many practical constraints, and offer pragmatic solutions that are easily implemented. Genetic Algorithm as one of the evolutionary algorithms has been employed to come up with an optimal number of capacitors (or distributed generation) and location in the distribution system. The method was chosen due to its robustness and its ability to explore all possible combinations on the solutions set, and finds optimal solution at reasonable amount of computation time. By deploying appropriate value of capacitors or distribution generators at suitable locations in the distribution systems, the losses can be reduced and hence obtain minimum total operational cost. The standard IEEE Node 13 Test Feeder

is the example used to demonstrate the feasibility of the technique.

### APPLICATION OF COMPLEX WAVELET TRANSFORM IN FREQUENCY ESTIMATION OF POWER SYSTEM

Jiaxin Ning Electrical and Computer Engineering Faculty Research Advisor: Dr. Wenzhong Gao

Frequency estimation is recently paid more attention since dynamic operations in the power system are required increasingly. Accurate frequency estimation plays a vital role in determining control schemes and performing real-time wide-area system protection. Many methods have been studied to estimate frequency, among which, Complex Wavelet Transform (CWT) provides a superior performance. Our objective is to improve the accuracy of the estimation with CWT, especially under the condition of dynamic frequency disturbance, and to extract more useful information from voltage/current signals. To evaluate our method, CWT is compared with conventional frequency estimation methods, such as classical Fourier Transform method and Four-parameter model method. The comparison results qualify CWT as an effective approach for frequency estimation.

### CONTINUUM MODELING OF LARGE ELECTRIC POWER SYSTEMS DURING FREQUENCY DISTURBANCES

### A. J. Thomas

Electrical and Computer Engineering Faculty Research Advisor: Dr. Satish Mahajan

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. There exist powerful, commercially available software packages designed to solve electromagnetic problems. It should be possible to apply all of the benefits that these packages provide to electromagnetism to continuum modeling, greatly simplifying the work. If continuum modeling becomes widespread, these software packages would have gained a new market.

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### HIGH VOLTAGE & HIGH CURRENT LABORATORY - IMPLEMENTATION AT TENNESSEE TECHNOLOGICAL UNIVERSITY

Diego M. Robalino Vanegas Electrical and Computer Engineering Faculty Research Advisor: Dr. Satish M. Mahajan

Electrical equipment suffers degradation due to long-term operation and eventual failures of the electrical system. The aim of this project is to provide an educational/research facility where High Voltage/High Power equipment were tested under conditions similar to those during real operation and emergency situations. Following the guidelines of highly recognized standards [1-6], the High Voltage (HV) & High Current (HC) Laboratory has been sequentially developed. The laboratory is capable of carrying out the condition assessment of electrical apparatus by means of DC (Direct Current) HV testing, Hot Spot Temperature (HST) measurement (via Fiber Optics and Thermocouples), HC Loading Set-up, Measurement and Protection Current Transformers Analysis, Tan  $\delta$ , permittivity, capacitance & Power Factor measurement via Insulation Diagnostic Equipment, Dielectric Breakdown Test and Online Dissolved Gas Analysis monitoring. This project greatly contributes to the development of research and academic opportunities for the TTU Electrical Engineering Department.

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### NEW CONTROL STRATEGY FOR FC-BATTERY HYBRID SYSTEM

### Ge Wang

Electrical and Computer Engineering Faculty Research Advisor: Dr. Wenzhong Gao

Proton Exchange Membrane (PEM) fuel cell shows great potential in both distribute generation and electric vehicles. In order to analyze dynamic characteristics of the fuel cell and perform control related studies, a 500W dynamic fuel cell model is built both in MATLAB/SIMULINK and VTB based on equivalent electrical circuit. Besides the three kinds of voltage drops due to activation loss, ohmic loss and concentration loss, the double layer charging effect and thermodynamics are also taken into account. This PEMFC model is valid and can be used for hybrid FC-battery system study. It has been commonly accepted that fuel cell is an excellent steady state source. However, it cannot respond to load transient as fast as desired. A battery is used to set up a FC-battery hybrid system to compensate the peak change of the load. The battery is modeled in MATLAB/SIMILINK based on experiment data. Our control strategy is to let fuel cell provide the steady-state power of the load and let the battery supply the peak power. Furthermore, when the state of charge (SOC) of battery drops below a certain limit, fuel cell will supply more power to charge the battery. The FC-battery system and its control loop are built in MATLAB/ SIMULINK, the simulation results demonstrate that the system works well and meet load demand.

### TIME REVERSAL ULTRA WIDEBAND SYSTEM TESTBED

Peng Zhang, Zhen Hu, and Yu Song Electrical and Computer Engineering, Center for Manufacturing Research Faculty Research Advisor: Dr. Robert Qiu

In the poster we will present our current research progress on ultra wideband (UWB) time reversal communication systems and channel sounding experiments results. We are building our second generation UWB test bed to demonstrate the time reversal concept using field programmable gate array (FPGA) based transmitter and

receiver. Based on the first generation test bed, we will add time reversal capability to perform channel compression, which will extensively reduce the complexity of the receiver design and improve the performance of the system in indoor environments. We will also show the measurement results of the channel sounding experiments in the rectangular metal cavity. Compared with the channel characteristics of hallway and office environments, confined metal environment shows significant difficulty in wireless communications. Exploring such characteristics guides us to design high performance wireless communication systems in many commercial and military applications.

### NEXA TRAINING SYSTEM

Vadim Zheglov

Electrical and Computer Engineering Faculty Research Advisor: Dr. Wenzhong Gao

Today's amounts of energy consumption require us to find new ways to generate energy and to make it easily accessible. Additionally, it has become obvious that the conventional energy generation using the fossil fuels is not sufficient enough to provide the mankind with required amounts. In the last decades the engineers worldwide have found ways to integrate the so called renewable energies into the power generation. One of the found concepts is the conversion of the chemical power into electrical power, which can be done by using fuel cells. The main focus of this project is to research ways of flexible and controllable applications of the Nexa training system. The heart of the training system is a modular 1.2 kW fuel cell. The additional integrated modules such as the power management module and the electronic load module make it possible to exanimate hydrogen supply via the electrochemical conversion in the fuel cell up to the electrical consumer. Practical simulations can be performed.

### INDUSTRIAL AND SYSTEMS ENGINEERING UNDERGRADUATE STUDENTS

### ERGONOMIC DESIGN OF POWERED HAND TOOLS FOR INSTALLING FASTENERS

Trey Bell Industrial and Systems Engineering Faculty Research Advisor: Dr. Jessica Matson

In today's manufacturing workplaces there are many powered hand tools being used incorrectly. Computer software, such as JACK, ergonomics analysis software, can help designers minimize the risk to operators while increasing productivity. The designed experiment will study the relation between productivity, operator comfort, and tool designs for tools designed to install screws. The design of the experiment will be such that the experiment can be repeated in future classroom settings and will allow students to better understand ergonomic concepts and the design of powered hand tools. The designed experiment will be compliant with current human subject's research guidelines.

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### MECHANICAL ENGINEERING GRADUATE STUDENTS

### PHASE FIELD MODELING OF CONTACT ANGLE HYSTERESIS IN SESSILE DROPS

Neeharika Anantharaju Mechanical Engineering Faculty Research Advisor: Dr. Mahesh Panchagnula Collaborator: Srikanth Vedantam (National University of Singapore)

Wetting on non-ideal surfaces is of great practical interest. Contact line behavior is an important parameter that attributes to understanding wettability. The presence of heterogeneities on a surface causes the pinning of the three-phase contact line in one of the many possible metastable states, resulting in contact angle hysteresis (CAH). CAH depends on the surface inhomogeneities, which are often random in size and position. The other factors like thermodynamic variables involved and the path followed makes quantifying the CAH challenging. Wetting of surfaces by sessile drops can thus be described as an interface phenomenon involving very steep changes at the contact line and is studied using a phase field model. The theory [1] uses a two dimensional non-conserved phase field variable to distinguish between wetted and non-wetted regions. The three-phase contact line tension is characterized by the gradient energy and CAH from the kinetic coefficient. A significant departure from the classical Cassie theory, arising due to the contact line pinning, is observed.

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### MODELING AND OPTIMIZATION OF AIR FLOW IN CABIN AIR FILTRATION TEST DUCT

#### Dhaman Kumar Besarla

Mechanical Engineering, Center for Energy Systems Research Faculty Research Advisors: Dr. Jie Cui and Dr. Sastry Munukutla

In many industrial applications, the cabin air test duct is used to test the efficiency and pressure drop of the filter. It is desired to have air flow as uniform as possible, as it comes to the filter in order to optimize its performance. The computational fluid dynamics (CFD) was used to simulate the cabin air filtration test duct. The velocity distribution of the test chamber obtained from numerical solution was validated against experimental results. A parametric study was carried out to identify the optimal design in terms of the uniformity of the velocity distribution at the test chamber.

### TURBULENCE MODELING OF TRANSIENT THERMAL MIXING

Murthy Lakshmiraju

Mechanical Engineering, Center for Energy Systems Research Faculty Research Advisors: Dr. Jie Cui and Dr. Sastry Munukutla

Transient thermal mixing induced by a sudden transverse injection of a fluid into a main flow of different temperature has many industrial applications. In this transient mixing process, a mixing region exists around and downstream of the injection point with high temperature gradients. The resulting thermal stresses and strain variations on the pipe wall can cause fatigue damage and cracking. Thus an understanding of this mixing phenomenon is vital. In the current research, numerical studies of the transient thermal mixing were carried out using various turbulence models to compare with the existing experimental data. The numerical results obtained were in good agreement with the experiments. Among the turbulence models, Large Eddy Simulation (LES) was found to produce more superior results in capturing the transient process of the thermal mixing. A parametric study was also performed to obtain temperature profiles under various flow and thermal conditions.

### NUMERICAL ANALYSIS OF TRANSIENT TEMPERATURE DISTRIBUTION IN A CURRENT TRANSFORMER

#### Mahesh Nadkarni

Mechanical Engineering, Center for Energy Systems Research Faculty Research Advisors: Dr. Jie Cui Current Transformer (CT) is a device that transfers the electrical energy from one circuit to another through a shared magnetic field. In a CT, heat is generated because of the energy losses in the core, tank wall, primary and secondary windings. The performance of the current transformer is well indicated by the temperature distribution inside a CT. In this study, numerical analysis is performed to predict the temperature distribution inside a CT at every instant under different load conditions. It is found that the numerical results obtained were in good agreement with the experimental measurements. Thus, it is concluded that the numerical method can be a useful tool in a CT design and performance monitoring.

### IMPROVING THE PROPULSION OF THE HUMAN POWERED SUBMARINE

Robert Porter Mechanical Engineering Faculty Research Advisor: Dr. Jie Cui

Computational fluid dynamic (CFD) software is used to do many industrial fluid mechanic investigations to verify models without the costly process of building prototypes. Recently the Tennessee Technological University human powered submarine team has been contemplating the use of a variable pitch propeller with the goal of increasing the acceleration of the submarine upon start up. In doing this the team generated several CFD simulations in order to investigate several theoretical aspects of the new propeller geometry. While the propeller blade airfoil shape was calculated using the analytical equations for standard NACA airfoils, CFD was used to investigate an optimal thickness that would give the best thrust without creating too much drag. CFD techniques were also employed to preliminarily investigate the performance of the variable pitch as compared to the fixed pitch that traditionally accounted for the thrust of the sub. This project seeks to describe the attempts of the team and document the finding of the CFD analysis.

### TURBULENT FLOWS THROUGH A CIRCULAR DUCT WITH A ROTATING FAN

Gaurav Vijay Rajwade Mechanical Engineering Faculty Research Advisor: Dr. Jie Cui

A fan is an important part for the circulation of air in household appliances and auto vehicles. To predict the fan performance, it is necessary to understand the resulting flow behavior. In this research an attempt has been made to extract this information using Computational Fluid Dynamics (CFD) technique. The objectives of this research are: 1) To produce the fan curve, which shows the relationship between air flow rate in the duct and the

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corresponding pressure drop. It is one of the most important information for fan selection. 2) To study the evolution of velocity profiles at various axial locations for different flow conditions. Preliminary results were found for a case with a stationary fan inside the duct and the data obtained was in good agreement with the experiment.

### A MATHEMATICAL MODEL TO PREDICT ELASTIC MODULUS OF NANOCOMPOSITE MATERIALS

Letchuman Sripragash Mechanical Engineering Faculty Research Advisor: Dr. John Peddieson

A continuum analytical model is developed to predict mechanical properties of nanocomposite materials with reinforcing nano-clay inclusions in a polymer matrix. Depending on the size distribution of the inclusions, the model developed herein assumes several different size inclusion phases imbedded in a matrix. The volume fraction of each phase is proportional to the volume fraction of the unique size inclusion in that phase. The elastic modulus of each phase can be estimated from Halpin-Tsai equations [1] and [2] and then using parallel and series configurations of all the phases, the resultant modulus is predicted. The model is compared with the available experimental data published in [3] and [4], and applied to created data having clearly defined properties. It is demonstrated that the distribution of inclusion sizes can have an important effect on elastic modulus predictions and that the trend of the predictions is in agreement with experimental data.

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### MECHANICAL ENGINEERING UNDERGRADUATE STUDENTS

### DYNAMICS OF LIQUID MARBLES

Kenneth C. Gahan and Prasad S. Bhosale Mechanical Engineering Faculty Research Advisor: Dr. Mahesh Panchagnula (Mechanical Engineering) Collaborator: Dr. Holly A. Stretz (Chemical Engineering)

Liquid marbles, which are water based liquids coated with a hydrophobic nanoparticulate substance resulting in small "marbles", are of interest to both chemical and mechanical engineers [1]. This study is motivated by the proposition that liquid marbles can provide for a rapid, contaminationfree transport mechanism of bio-fluids. The current research seeks to understand the unique manner in which liquid marbles behave under dynamical conditions. Under rolling motion, liquid marbles are observed to behave differently from solid spheres in that they accelerate quickly before settling to a terminal velocity, due to the damping effects of the liquid core [2].

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### ACKNOWLEDGEMENTS

#### ACKNOWLEDGEMENTS

The Research Day Committee gratefully acknowledges everyone who contributed in any way to the success of Student Research Day 2008. The day's activities are designed to showcase student research and the great deal of activity that is currently underway on campus. A total of 108 abstracts involving ~114 undergraduate and graduate students, more than 40 faculty advisors, and various collaborators both inside and outside TTU were received for presentation this year from a number of departments across campus.

The event would not be possible were it not for the collective energies, dedication, and initiative of MANY individuals, departments, and other groups across campus. Of particular note, thank you to Monica Greppin in Public Affairs for her guidance and assistance with advertising the event; to Dewayne Wright for coordination of publication activities and to James Mabery and Lorie Worley for the design and preparation of this booklet and cover. Also, we wish to thank Dean Carothers in Photo Services for preparing the display boards and for his assistance with photographing the day's events. Thank you to Printing Services for timely printing of this booklet. The Committee further recognizes the University Bookstore and University Dining Services for the role that each has played with this activity.

We extend sincere thanks and appreciation to Dr. Allen Atkins and Boeing Corporation for monetary awards for the best posters and also to David and Sherri Nichols for their endowment to support Student Research Day activities.

The bronze medallions that will be provided for the best posters were designed and manufactured as part of a senior research project by students (Jacob Burkey, Stephen Gallagher, Stephen Goodman, and Christopher Nabors) in Dr. Ahmed ElSawy's Manufacturing and Industrial Technology class. We are extremely grateful to them for the significant contributions that they all made and to the TTU Chapter of the Sigma Xi Scientific Research Society for co-sponsoring this activity.

We would also like to thank President Bell and Provost Armistead for their support of this event. Faculty, department chairs, college deans, and center directors all provided valuable contributions to ensure the success of the day's events. A special thanks is extended to Mark Lynam, Kathy Reynolds, Sammie Sparks, and Ellen Wolfe in the Office of Research for excellent assistance and services provided in making this event a reality.

To all who helped in any way listed or not, THANK YOU VERY MUCH!

Most sincerely,

The Research Day Committee Dr. Pat Bagley Dr. Subramaniam Deivanayagam Dr. Virginia Moore Dr. Paul Semmes Dr. John Wheeler Dr. Robby Sanders Dr. Francis Otuonye

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