

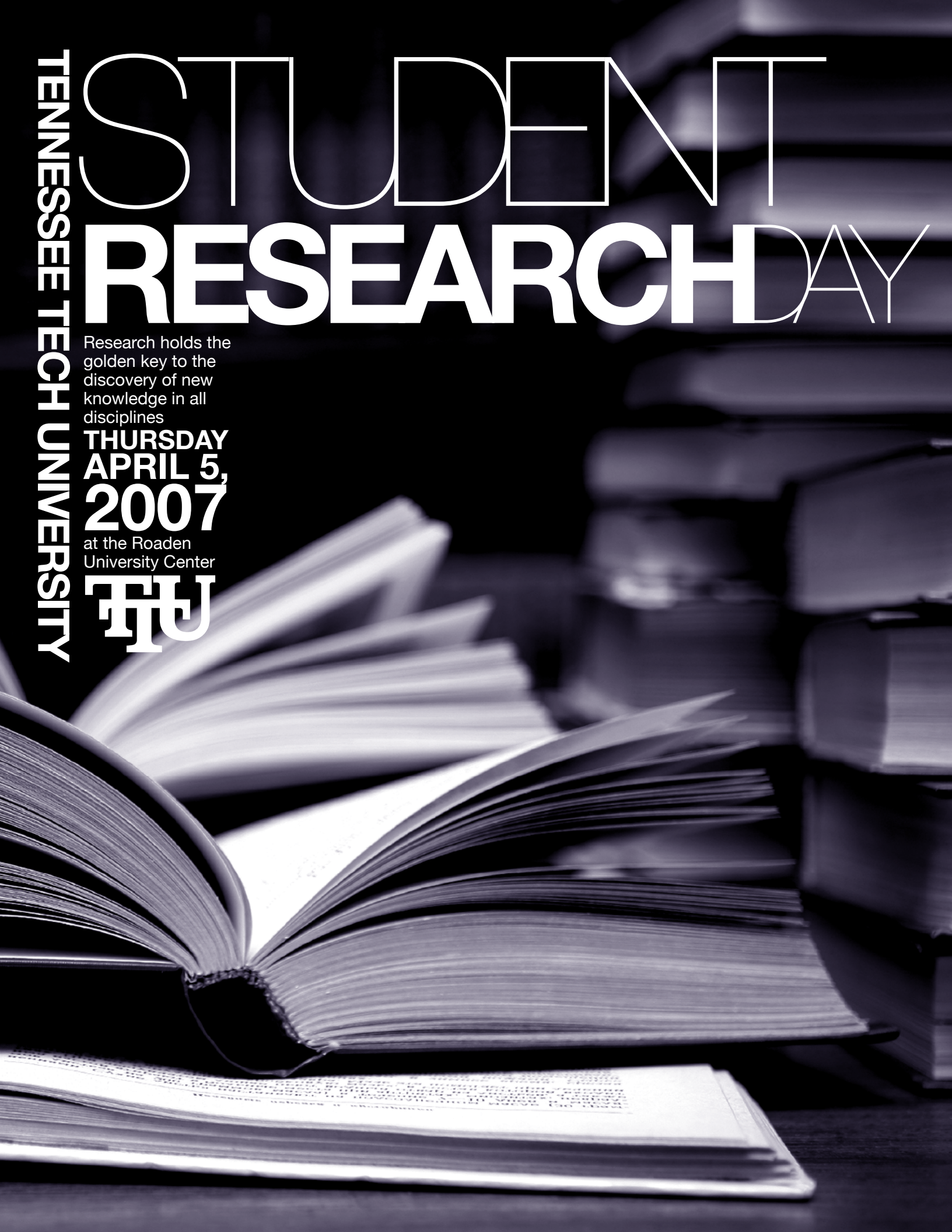
TENNESSEE TECH UNIVERSITY

# STUDENT RESEARCH DAY

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

**THURSDAY  
APRIL 5,  
2007**

at the Roden  
University Center



# CHEMICAL ENGINEERING GRADUATE STUDENT

## DETERMINATION OF STRAIN STATES IN ORDINARY PORTLAND CEMENT USING NEUTRON DIFFRACTION

Sean E. Mikel

Chemical Engineering

Faculty Research Advisor: Dr. Joseph J. Biernacki

Collaborator: Thomas Gnaeupel-Herold (NIST Center for Neutron Research)

Neutron diffraction techniques have been applied for the determination of strain and residual strain in hydrated portland cement paste. Strains were induced by uniform, compressive, uniaxial, mechanical loading. The neutrons were used to make in-situ measurements of the interplanar spacing of the calcium hydroxide (CH) phase within the neutron beam path of the cement specimen. Results show a nominally linear relationship between the applied load and the diffracting interplanar crystal spacings. In addition, compressive residual strain was observed in the cement samples in the “unloaded” state when compared to the theoretically relaxed powder samples. Neutrons penetrate deep within the sample and diffraction can be observed in transmission mode. This provides a meso-scale volume from which diffraction occurs. The data from this study is very encouraging and may prove to be an invaluable tool in the determination of phase resolved multi-scale mechanics in ordinary portland cement and other cementitious materials.

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## **AWARDS ACKNOWLEDGEMENTS**

Medallion awards were designed and manufactured by the following students in Manufacturing and Industrial Technology: Ryan Black, Mark Copeland, Walter Keen, Roderick Macleod.

A monetary award is being made in recognition of those presenting the best posters in each discipline during Student Research Day. It is provided through the generosity of Dr. Allen Atkins (TTU Alumnus) and Boeing.

# TABLE OF CONTENTS

■ Research Day Purpose .....	2
■ Schedule of Events.....	2
■ A Message from the President.....	3
■ A Message from the Provost.....	4
■ A Message from the Associate Vice President for Research.....	5
■ Student Abstracts .....	6-26
■ Arts and Sciences.....	6-11
Chemistry .....	6
Computer Science .....	6-10
Mathematics.....	10
Physics .....	11
■ Education.....	12
■ Engineering.....	13-26
Chemical Engineering.....	13-19
Civil and Environmental Engineering .....	19-20
Electrical and Computer Engineering .....	21-23
Industrial and Systems Engineering .....	23-24
Manufacturing and Industrial Technology .....	24
Mechanical Engineering .....	24-26
■ Acknowledgements.....	26
■ Directory of Participants.....	27
■ Notes and Comments .....	28

# RESEARCH DAY - PURPOSE

Research and Instruction are equal partners in the Academy. Knowledge is imparted to students via instruction by the faculty with the hope that the students will be motivated to learn more. The quest for increased knowledge is the way we define research, thereby making it a perfect complement to instruction.

The purpose of RESEARCH DAY is to demonstrate the importance of research or inquiry in instruction and to show that instruction and research are indeed complementary. The freedom of inquiry and/or investigation is at the very nucleus of training in the Academy. Research is the component that gives real meaning to instruction.

RESEARCH DAY is a display of the SCHOLARSHIP students – both graduate and undergraduate- possess as manifested by the sharing of new knowledge gained through inquiry under the tutelage of Faculty Research Advisors.

The poster presentations give students experience in condensing a body of factual information to a few salient points without loss of meaning.

## SCHEDULE OF EVENTS

### Student Research Day

Roaden University Center  
Multipurpose Room

**Thursday, April 5, 2007**

- 7:00 a.m. – 7:45 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 5, 2007

Dear Student Investigators:

On behalf of the students, faculty and staff at Tennessee Technological University, I offer my congratulations and appreciation to you for the quality research you have accomplished under the guidance of your faculty research advisors. You bring honor and recognition to yourself, the University, the greater community and to the State through your participation in the scholarly activity of sharing your new knowledge.

Research is at the heart of University training. The type of scholarship displayed by you today through your poster presentation has contributed significantly to Tennessee Technological University being named one of the Best Southeastern Colleges by The Princeton Review and one of the South's Best Universities-Master's Level by U.S. News & World Report.

Thank you for participating!

Sincerely,



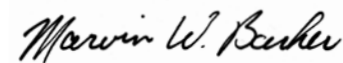
Robert R. Bell  
President

Dear Tennessee Tech Students:

Whether you are a graduate or undergraduate student, research experiences will provide you with leading-edge learning and knowledge acquisition. That is why this University values and supports research activities by students.

Welcome to "Student Research Day." This and future Research Days are designed to showcase the excellent research and scholarly activity by students and to disseminate the results.

Sincerely,



Marvin W. Barker  
Provost and Vice President for Academic Affairs

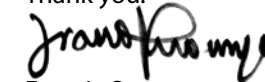
#### WELCOME TO TENNESSEE TECH RESEARCH DAY

It is with great pleasure that the staff of the Office of Research and Graduate Studies welcomes you to the Student Research Day. Today, students from the different disciplines on our campus showcase the research that they have conducted under the leadership and guidance of their professors. The projects are a glimpse of the different types of scholarly activities that take place at Tennessee Technological University.

Our vision of commitment to the life-long success of our students is enhanced through participation in research. 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 technology is developed and transferred to benefit society.

On behalf of the Research Liaison Officers for their roles in planning and encouraging participation in the Student Research Day, we express our appreciation to the students who have presented their posters, and to the faculty advisors who have supervised and guided the projects. We are very excited by the opportunity provided by the Student Research Day, and we hope that the projects would generate 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



## CHEMISTRY GRADUATE STUDENTS

### THEORETICAL INVESTIGATION OF A HYDROGEN ABSTRACTION FROM FLUOROETHANES BY HYDROXYL RADICAL

N. W. S. V. Nuwan De Silva  
Chemistry  
Faculty Research Advisor: Dr. Titus V. Albu

Geometric and energetic parameters for the hydrogen abstraction reaction of fluoroethanes by the hydroxyl radical were obtained using new hybrid density functional theory methods. In this study geometries of all stationary points along the reaction path (the reactants, transition states and products) involved in hydrogen abstraction reactions of CH<sub>3</sub>CH<sub>2</sub>F (HFC-161), CH<sub>3</sub>CHF<sub>2</sub> (HFC-152a), CH<sub>2</sub>FCH<sub>2</sub>F (HFC-152), CH<sub>3</sub>CF<sub>3</sub> (HFC-143a), CH<sub>2</sub>FCHF<sub>2</sub> (HFC-143), CH<sub>2</sub>FCF<sub>3</sub> (HFC-134a), CHF<sub>2</sub>CHF<sub>2</sub> (HFC-134), CHF<sub>2</sub>CF<sub>3</sub> (HFC-125) with OH radical were optimized at three different hybrid density functional theory methods mPW1B95-31, mPW1B95-38, mPW1B95-44 used for comparison aims in conjunction with the 6-31+G(d,p) basis set. Our results show that the mPW1B95-44 /6-31+G(d,p) method gives the best results for energetic parameters including barrier heights and transition state geometries.

### A THEORETICAL INVESTIGATION ON THE ISOMERISM AND THE NMR PROPERTIES OF THIOSEMICARBAZONES

N. W. S. V. Nuwan De Silva  
Chemistry  
Faculty Research Advisor: Dr. Titus V. Albu

Hybrid density functional theory calculations at the mPW1PW91/6-31+G(d,p) level of theory have been used to investigate the optimized structures and other molecular properties of five different series of thiosemicarbazones. The investigated compounds were obtained based on acenaphthenequinone, isatin and its derivatives, and alloxan. The focus of the study is the isomerism and the NMR characterization of these thiosemicarbazones. It was found that only the one isomer is expected for thiosemicarbazones and methylthiosemicarbazones, while for dimethylthiosemicarbazones, two isomers are possible. All investigated thiosemicarbazones exhibit a hydrazinic proton that is highly deshielded and resonates far downfield in the proton NMR spectra. This proton is a part of a characteristic six-membered ring, and its NMR properties are a result of its strong, intermolecular hydrogen bond. The relationships between the calculated <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts and various geometric parameters are reported.

## COMPUTER SCIENCE GRADUATE STUDENTS

### REQUIREMENT DEFECTS DISCOVERY AND ANALYSIS IN AN ACADEMIC ENVIRONMENT

Michael Baldwin  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

Development of the Software Requirements Specification (SRS) document is a critical task in the software development process as these requirements set the basis for further system development and overall project cost and schedule estimation. [1] The focus of this research study is to identify the most frequently occurring defects, i.e., any deficiency that can affect the development process [2], in requirements specification documents developed by students conducting class term projects on system software development in an academic environment. The study itself consists of taking the set of SRS documents and inspecting them to locate requirements defects utilizing a checklist, based on the one described in [3]. The results of this study will identify checklist items most relevant to student projects in an academic setting and help to develop a new checklist better suited in such environment.

#### References

1. T. Javed, M. e Maqsood, and Q. S. Durrani, "A study to investigate the impact of requirements instability on software defects." SIGSOFT Software Eng. Notes, vol. 29, no. 3, pp. 1-7, 2004.
2. Conrad M. Gel properties of egg white. J. Food Sci. 2002; 67: 725 – 728.
3. A. Siraj, "A software inspection checklist based on IEEE recommended practice for software requirements specifications."

## DISTRIBUTED SYSTEM FOR RECORD LINKAGE GOLD STANDARD GENERATION

Jeremy Ey and Andrew Walker  
Computer Science  
Faculty Research Advisor: Dr. Doug Talbert

Record linkage is the process used to create associations between records in disjoint record sources. This technique has many applications [1,2,3], one example is the linkage of medical records from various hospitals to form a more complete view of an individual's medical history [4]. The proper evaluation of the algorithms requires measuring the performance of the algorithm over a set with known links. This set is referred to as a gold standard set. These sets are often hand produced. This leads to sets that are either too small or nonexistent [5]. The need to easily produce gold standard data sets has motivated the development of a distributed deterministic rule engine. This system allows for the specification of deterministic rules which are used to produce a gold standard data set. This gold standard set can then be compared to the results produced by implementations and enhancements of record linkage algorithms.

#### References

1. Clark, D. E. Practical introduction to record linkage for injury research. Injury Prevention 10, 3 (2004), 186–191.
2. Fuller K. No-cream ice creams. Better Homes and Gardens. 1996; 74:228.
3. Winkler, W. The state of record linkage and current research problems. RR99/03, US Bureau of the Census (1999).
4. Working Group on Accurately Linking Information for Health Care Quality and Safety. Linking health care information: proposed methods for improving care and protecting privacy. Markle Foundation, February 2005.
5. Tromp, M., Reitsma, J., Ravelli, A., Meray, N., and Bonsel, G. Record linkage: Making the most out of errors in linking variables. In AMIA Symposium Proceedings 2006 (2006), pp. 779–783.

## GLOBAL SOFTWARE DEVELOPMENT WITH EXTREME PROGRAMMING

Chandra Sekhar Jamalpur  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

In today's highly competitive market, Global software development (GSD) [1] is increasingly becoming a common practice in the software industry. It allows software development at remote sites ignoring their geographical distance and embracing benefits from availability of vast qualified resource pool and reduction in development costs. Agile software development [2] is a latest approach to software development which focuses on lightweight

processes and adaptability to change. The most widely practiced agile methodology is eXtreme Programming (XP) [3], which offers a great way of monitoring and controlling rapid product development cycles. While XP offers features that are potentially useful for GSD, GSD is distributed in nature and it appears to contradict XP practices in many ways. This research will investigate the challenges involved in XP practices in the context of GSD and suggest guidelines to resolve issues of concerns.

#### References

1. Christof Ebert., et al., "Surviving Global Software Development," IEEE Software 18(2): 62-69 - (2001).
2. High smith, J., Cockburn, A., " Agile software development the business of innovation," Computer - IEEE CS Press, Volume 34, Issue 9, Sept. 2001 Page(s):120 – 127.
3. K. Beck, Extreme Programming Explained Embrace Change, Addison-Wesley Longman, Inc., 2000.

## TRACKING SECURITY THREAT SCENARIOS FOR DEFENSE

Brandon Malone  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

As web-centric applications gain popularity, security threats originate from more subtle sources than ever before [1]. Misuse cases, which portray potential dangers to proper system functioning, effectively model many of these threats [2]. However, as these abstract representations flesh out into more thorough design details, the high-level rationales behind security features may remain stranded with the initial requirements. Without such justifications, these crucial characteristics may simmer on the implementation backburner as flashy features hog the development budget. Tracking the security defenses does not come for free, though: strategies akin to those following the refinement of functional requirements into system design must also track architectural decisions influenced by security threats [3]. This research proposes some simple UML extensions to follow the honing of misuse cases into design elements, and ultimately into lines of code.

#### References

1. Van der Stock, Andrew, ed. A Guide to Building Secure Web Applications and Web Services. 2.0 Black Hat Open Web Application Security Project. 2005.
2. Sindre, Guttorm, and Andreas Opdahl. "Capturing Security Requirements through Misuse Cases." NIK 2001, Norsk Informatikkonferanse 2001. 2001.
3. Kean, Liz. Requirements Tracing - An Overview. February 1998. [http://www.sei.cmu.edu/str/descriptions/reqtracing\\_body.html](http://www.sei.cmu.edu/str/descriptions/reqtracing_body.html).

## COMPUTER SCIENCE UNDERGRADUATE STUDENTS

### OSCAR PACKAGE SETS

Wesley Bland  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

Collaborators: Thomas Naughton, Geoffrey Vallee, and Stephen L. Scott (Oak Ridge National Laboratory)

A cluster is a dedicated group of computers working together. For creating and maintaining such a cluster in Linux environment, OSCAR (Open Source Cluster Application Resources) is often used, which combines many of the most popular applications in this environment. Currently, there are many different "flavors" of OSCAR including High Availability and Diskless, and a need for a package set system to simplify the installation. By creating a "package set", different flavors of OSCAR could essentially be combined into a single version, making OSCAR installation much simpler and more flexible for current users. The new package set system for OSCAR would divide up the different flavors of OSCAR and resolve any conflicts or requirements that may arise in doing so. It would then be incorporated into the main OSCAR code and be released for use with future versions of OSCAR.

### SPAM PROFITABILITY COUNTERMEASURE

Sam Bledsoe  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

Spams are unsolicited universally undesired electronic messages. Spam marketers rely on 1) very low cost per exposure and 2) miniscule response rates to operate profitably [1]. This research intends to test a method of active response to this problem that has been practically unstoppable thus far. Invalidating the above mentioned conditions has the potential to make spam economically impractical for those seeking marketing. To this end we aim to use the user response rate, which depends completely on actions of spam recipients, against the profitability of the spam marketers. This research will produce software for the individual spam recipients that will operate on their behalf to increase their own response rate, and evaluate the results. The final goal is contributing in increasing the spammers' costs for monthly bandwidth quotas and the time spent in searching for valid responses, thus acting as a deterrent for the spam marketers.

#### Reference

1. [http://en.wikipedia.org/wiki/Spam\\_\(electronic\)](http://en.wikipedia.org/wiki/Spam_(electronic))

### INTERNET STALKING: AN ANALYSIS OF A LEADING SPYWARE PROGRAM

Robby Florence  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

Spyware has become one of the fastest growing internet security threats over the past few years. It is computer software that collects personal data without the user's consent. The data is then transmitted to marketing organizations or some other unauthorized agency (Edelman). Spyware can also affect the user's computer with decreased performance, pop-up ads, or changed internet settings. There are a few prominent spyware producers in the market whose advertising software is installed on millions of computers (eTrust). These spyware programs track the user's browsing habits, display frequent pop-up advertisements, and slow system performance, often without users even knowing they are installed (PCPitstop). This research will look into the security issues concerning one of these popular spyware products and investigate: how it makes its entry into a computer, how it collects information, what it can collect, and how to get protection from it and eradicate it from one's computer.

#### References

1. Edelman, Benjamin. "Spyware": Research, Testing, Legislation, and Suits. <http://www.benedelman.org/spyware/>
2. eTrust Spyware Encyclopedia - Claria. <http://www3.ca.com/securityadvisor/pest/pest.aspx?id=453088629>
3. PCPitStop Gator Information Center. <http://www.pcpitstop.com/gator/default.asp>

### ADDING SECURITY IN UNIX: HAS IT HELPED?

Kyle Guillot  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

UNIX is a very widely known and utilized operating system. Its original design did not incorporate security, but because of the emerging and critical need, UNIX has gone through some evolution in the context of security. This research will investigate how effective the addition of security to UNIX has been, as opposed to building it into an operating system. Specifically, the topics covered will be: information and statistics about known vulnerabilities and patches (Loukides et al. 48.3), the danger of the superuser concept in UNIX, and exercising security features in an UNIX based system (Garfinkel et al.).

#### References

1. Loukides, Mike, Tim O'Reilly, Jerry Peek, and Shelley Powers. UNIX Power Tools. 3rd ed. 2 Nov. 2002.
2. Safari Books Online. 14 Feb. 2007. <<http://proquest.safaribooksonline.com/0596003307>>.

### INVESTIGATING VISTA'S SECURITY VIBES

Matt Hermanson  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

This research will investigate the security features that are included in the new Windows operating system, Vista. Along with better graphics and more functionality, security has been one of the major selling points of Vista(1). Microsoft claims to include user account control, authentication, anti-malware, network access protection, firewall, windows service hardening, internet explorer enhancements, and data protection as the primary features to make Vista so appealing(1). However, some Vista skeptics have already placed doubt that while impressive, it is not yet worth its hefty price tag(2). Vista also brings with it some more than modest system requirements. The average user will require an upgrade various hardware areas, maybe even a new computer all together, which only tacks onto the price of upgrading(3). The research question we want to investigate is how much one is willing to pay for sense of security and whether it pays off.

#### References

1. <http://technet.microsoft.com/en-us/windowsvista/aa905073.aspx>
2. <http://redmondmag.com/columns/article.asp?EditorialID=1621>
3. John Clyman. "The insiders guide to Windows Vista". PC Magazine. December 20th, 2006.

### AUTOMATION OF MOBILE AGENT IN ELECTRONIC MARKET

Viatcheslav A. Meisner  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

The mobile agent paradigm has wide range of applications like: network management, data-mining, and online auctions. This research focuses on the use of mobile agents in electronic market for trading purposes. Particularly we look at the Consumer Buying Behavior model [1], which describes need identification, product brokering, merchant brokering, negotiation, purchase and delivery, and service and evaluation phases of buying process. This research will investigate automation of mobile agent's role in the buying and selling process, particularly on the negotiation phase and suggest a working protocol in this regard.

#### References

1. Robert H. Guttman, Alexandros G. Moukas, and Pattie Maes, "Agent-mediated Electronic Commerce: A Survey." Software Agents Group, MIT Media Laboratory, 20 Ames street, E15-305, Cambridge, MA 02139.

### DESIGNING FOR THE MOBILE WEB – STANDARDS AND BEST PRACTICES

Derek Pennycuff  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

This research targets availability of Cascading Style Sheet media support in a variety of mobile devices. The World Wide Web Consortium's specifications for various web standards document how mobile browsers should behave. Designing based on these standards without testing or documentation on their support proves impossible even in more traditional devices. Testing on all possible mobile platforms is impractical. A baseline level of documentation could lead to a list of best practices when designing for mobile devices. This research seeks to contribute to that documentation with a sampling of cell phones, personal digital assistants, and hand held gaming systems. The research methodology will involve loading in the web browsers of the available hardware a compact test case consisting of all the necessary test criteria and recording the results. These results will be compared against the published standards and analyzed to report the extent of any deviations found.

### SECURITY WEAKNESSES IN WIRELESS NETWORKS

Michael Rohling  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

The security of wireless networks has become a growing public concern as wireless access points become increasingly ubiquitous. It was discovered early on that the most common encryption standard, WEP (Wired Equivalent Privacy), was vulnerable to attack from an intruder who could capture enough packets to determine the encryption key.1 Newer, stronger encryption standards came into use in later generation products, but these too were also found to be vulnerable to a dedicated intruder.2 Although wireless networking cannot be made completely secure, there are precautions that may be taken in order to deter most attackers. This research will attempt to determine the viability and effectiveness of popular attacks against wireless networks by attempting them in order to suggest some measures that can be used to thwart would-be intruders.

#### References

1. [http://en.wikipedia.org/wiki/Wired\\_Equivalent\\_Privacy](http://en.wikipedia.org/wiki/Wired_Equivalent_Privacy)
2. [http://en.wikipedia.org/wiki/Wi-Fi\\_Protected\\_Access](http://en.wikipedia.org/wiki/Wi-Fi_Protected_Access)



## WEBSITE SECURITY: INVESTIGATING SECURITY LOOP HOLES

Robert Wilkinson III  
Computer Science  
Faculty Research Advisor: Dr. Ambareen Siraj

Much of our daily routines involve information exchange in our current technologically driven world, which is in some way connected to the internet. A copious amount of personal and organizational information flows throughout this system. One access point to this information is via a website. With every new day comes a new security threat. This notion exemplifies the relentlessness of attackers in this highly technical society and websites are no exception. Attention to the current security vulnerabilities related to websites is needed because the first step in securing these threat areas resides in understanding the vulnerabilities themselves. This research covers one of the most extensively exploited areas, cross-site scripting[1], as well as other common vulnerabilities including session hijacking, multiple forms of code injection, cross zone scripting and cross-site request forgery. Knowledge of these loop holes will result in more concern for website security and ultimately lead to a safer system.

### Reference

1. Ollmann, Gunter. "Understanding the cause and effect of CSS (XSS) Vulnerabilities," Technical Info, <http://www.technicalinfo.net/papers/CSS.html>, Feb. 13, 2007.

## MATHEMATICS GRADUATE STUDENTS

### HIERARCHICAL MATRIX BASED SMOOTHER FOR THE MULTIGRID METHOD

David Priebel  
Mathematics and Computer Science  
Faculty Research Advisor: Dr. Sabine Le Borne

Hierarchical matrices are a class of matrices that are well suited to represent sparse data and provide almost linear complexity operations[1]. In particular, the cost of computing the approximate LU decomposition of a hierarchical matrix is relatively inexpensive[2]. This fact makes it possible to apply H-matrices to the problem of smoothing the error of intermediate approximate solutions. Using the H-matrix based method as a smoother for the Multigrid Method results in an improved convergence rate. We have implemented the Multigrid Method with H-matrix smoothing and provide a numerical study of robustness for a variety of test problems.

### References

1. Wolfgang Hackbusch. A sparse matrix arithmetic based on H-matrices. Part 1: Introduction to H-matrices. *Computing*, 62(2):89-108, 1999.
2. S. Le Borne, L. Grasedyck. H-matrix preconditioners in convection-dominated problems. *SIAM J. Matrix Anal. Appl.*, 1172-1183 (2006).

## MATHEMATICS UNDERGRADUATE STUDENTS

### NEW MATHEMATICAL TECHNIQUES FOR COMPUTATIONAL FLUID FLOW SIMULATION

David W. Cook II  
Mathematics and Computer Science  
Faculty Research Advisor: Dr. Sabine Le Borne

Mathematically modeling how fluids flow in an environment is important, allowing for simulations of situations that have prohibitive costs and dangers involved; further, situations which are simply impossible to test in real laboratory experiments can also be simulated. These models often lead to the formation of saddle point systems. Recently, a large amount of research has been devoted to finding more efficient methods for solving systems of equations—saddle point systems, in particular. However, finding techniques which scale up to larger problems with a minimal increase in requirements is a daunting task. We have developed a novel factorization technique H-QR in [1] which allowed the development of a new and widely applicable solver for saddle point problems. The originality of this solver is based on the combination of the well-known null space method with the recently discovered technique of hierarchical matrices.

### Reference

1. Sabine Le Borne and David W. Cook II. Construction of a discrete divergence-free basis through orthogonal factorization in H-arithmetic. Submitted for publication, 2007.

## PHYSICS UNDERGRADUATE STUDENTS

### A DATA ACQUISITION SYSTEM FOR NU-SNS DEVELOPMENT

S.V. Paulauskas  
Physics  
Faculty Research Advisor: Dr. Raymond L. Kozub

### Collaborators:

J.C. Blackmon, Qinglin Zeng, Dan Bardayan (ORNL)  
Y.V. Efremenko (Univ. Tennessee at Knoxville)  
K. Scholberg, A. Cromwell (Duke Univ.)

The nu-SNS project at the Spallation Neutron Source aims to study neutrino-nucleus interactions important for understanding nuclear structure and astrophysics. Understanding the neutron background produced by the 1 GeV proton beam of the SNS is crucial to designing the shielding and detectors for nu-SNS. To this end a facility is being constructed to study the neutron backgrounds at the SNS. In order to process data from scintillation detectors a LabVIEW [1] program was written. This program communicates with CAMAC based ADC modules via a GPIB crate controller and a USB interface. Three of the ADCs receive gates to store information from different time intervals for neutron-gamma discrimination. The fourth ADC stores TAC signals with neutron TOF information. The LabVIEW [1] program creates spectra that can be used to identify neutrons and gamma rays. Measurements with neutron and gamma sources were performed to study the effectiveness of different techniques of neutron-gamma discrimination.

### Reference

1. LabVIEW is a trademark of National Instruments Corporation.

### LIMITATIONS AND IMPROVEMENT OF THE GAMOW WINDOW APPROXIMATION FOR THERMONUCLEAR REACTION RATES

J. Tokiwa  
Physics  
Faculty Research Advisor: Dr. Raymond L. Kozub

### Collaborators:

M. S. Smith (ORNL)  
J. P. Scott, E. J. Lingerfelt, K. Chae (ORNL/UT-Knoxville)

The knowledge of thermonuclear reaction rates is vital to simulate numerous types of astrophysical events. Standard codes to calculate rates, such as the tools at [nucastrodata.org](http://nucastrodata.org), utilize a Gaussian approximation [1] to estimate the relative energy range (Gamow window) over which the calculation is performed numerically. This approximation fails by returning an energy range that extends to negative values for some reactions involving low Z particles at low temperatures, such as the  $d(d, n)^3\text{He}$  and  $d(d, p)t$  reactions, which are important for Big Bang Nucleosynthesis. A new code has been written to numerically determine the energy range for the calculation needed to obtain an accuracy of less than 1% in the reaction rate, based on rate contributions from various energies in the Gamow window at a given temperature. This extends the rate calculation capabilities at [nucastrodata.org](http://nucastrodata.org) to include Big Bang Nucleosynthesis. This research is supported by the U.S. Department of Energy under grants DE-AC05-00OR22725 (ORNL) and DE-FG02-96ER40955 (TTU).

### Reference

1. See, e.g., C. E. Rolfs and W. S. Rodney, "Cauldrons in the Cosmos," The University of Chicago Press, Chicago (1988), p. 158.



## GRADUATE STUDENTS

### PURSUING DIAGNOSIS FOR CHILDREN WITH ASPERGER SYNDROME: PARENTS' PERSPECTIVES

Xiuchang Ann Huang  
Education  
Faculty Research Advisor: Dr. John J. Wheeler

Late diagnosis in children with Asperger syndrome (AS) is common. The purpose of this qualitative study is to reveal the parents' experiences and perspectives of pursuing diagnosis for their children with AS in order to assist other parents' of children with similar symptoms in pursuing diagnosis earlier and more successfully. The major research method is semi-structured interview. Parents from 8 families participated in this study. Data were coded and categorized first and then were analyzed using constant comparison method. Finally conclusion was made and recommendations were provided.

### TEACHING EMOTION RECOGNITION TO A CHILD WITH ASPERGER SYNDROME

Xiuchang Ann Huang  
Education  
Faculty Research Advisor: Dr. John J. Wheeler  
Collaborator: Dr. Michael Mayton (Curriculum & Instruction)

Children with Asperger syndrome (AS) have poor emotion awareness and recognition (Solomon, Goodlin-Jones, & Anders, 2004). Poor emotion awareness & recognition result in impairments in reciprocal social interaction in this population (Attwood, 1998). Since few studies look for solutions to solve this problem, this case study aims to enrich existing literature by developing an intervention to improve this ability of a 10-year-old boy with AS who has difficulty in recognizing others' emotional states. Changing criterion design is used to measure his progress across training sessions. Results show the participant has distinct difficulty in discriminating complex emotion states (e.g., afraid/worried and surprised); his performance is closely related to his attention span; and his emotion recognition ability improves dramatically after the training. The study concludes that individuals with AS can learn to identify emotion states correctly if they are taught systematically.

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## CHEMICAL ENGINEERING GRADUATE STUDENTS

### AQUEOUS HYDROGEN FLUORIDE MIXTURE – FROM CLUSTERS TO BULK

Barath Baburao  
Chemical Engineering  
Faculty Research Advisor: Dr. Donald P. Visco, Jr.  
Collaborator: Titus V. Albu (Chemistry)

In an attempt to understand the phase behavior of aqueous hydrogen fluoride, we study the mixture from the molecular level and use that information to correlate and predict the properties in the bulk-phase. A bulk-phase association based thermodynamic model was developed for both the pure components and mixtures. This model was extended to mixtures, with considerations for both self and cross-association. To gain a perspective on the several complex association patterns that is present in this mixture, a molecular level study was performed using mPW1B95 [1], a recently developed hybrid meta density functional theory method. We study the stable geometries of the clusters of  $(\text{HF})_n - (\text{H}_2\text{O})_m$  with  $m+n$  up to 8. For each cluster type, several different structures are investigated, and the most stable structure for each cluster is reported based on the electronic and Gibbs free energy values. These association patterns are in turn included in the bulk-phase thermodynamic model and used to correlate and predict the properties of this industrially important mixture.

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### ORDERED NANOLAYERS OF CERAMIC NANOPARTICLES

Prasad S. Bhosale  
Chemical Engineering  
Faculty Research Advisor: Dr. Holly Stretz

Postsynthesis processing of nanoparticles in polymer nanocomposites to obtain meso- and bulk scale hierarchical structures remains a challenge for nanotechnology and for smart materials development. This work is to investigate a coating processes to achieve ordered arrays of anisotropic, high modulus nanoparticles ceramic nanoparticles like fumed silica and montmorillonite clay nanoparticles which contribute a combination of stiffness, wear resistance and thermal stability to the final material. While ordered

arrays of nanoparticles are reported often in the literature [1-3], the results are generally for spherical gold and silver-type nanoparticles, and to our knowledge deposition of anisotropic, high modulus particles on polymer surfaces (outside of carbon nanotubes) is not well understood. In particular this study is focused on the deposition by layer by layer deposition [4], nanoparticle self assembly processes [5] and CO<sub>2</sub> expanded liquid deposition [6].

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### TOWARDS REAL-TIME (MILLI-SECONDS) SIMULATION OF PHYSICS BASED LITHIUM-ION BATTERY MODELS

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

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. Mathematical modeling [1-3] of lithium-ion batteries involves the specification of the dependant variables of interest (for e.g., solution phase potential), the first principles based derivation of governing equations for these dependant variables and specifying the boundary and initial conditions for these governing equations. 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. Rigorous physics based models take up to few minutes to simulate discharge curves depending on the solver, routines, computers, etc. This poster presents an effective approach [4-5] to simulate physics-based lithium-ion battery models in real-time (milli-seconds) for simulation and control in hybrid environments.

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### IN<sub>0.1</sub>SN<sub>0.9</sub>P<sub>2</sub>O<sub>7</sub>-NAFION COMPOSITE MEMBRANE FOR DMFC

Bin Fang and Jian Hong  
Chemical Engineering  
Faculty Research Advisor: Dr. Chunsheng Wang

A high proton conductor In<sub>0.1</sub>Sn<sub>0.9</sub>P<sub>2</sub>O<sub>7</sub> was dispersed in Nafion polymer to form an In<sub>0.1</sub>Sn<sub>0.9</sub>P<sub>2</sub>O<sub>7</sub> - Nafion composite membrane [1]. The performances of Direct Methanol Fuel Cell with In<sub>0.1</sub>Sn<sub>0.9</sub>P<sub>2</sub>O<sub>7</sub>-Nafion composite membranes were investigated in a wide temperature ranges (from 30 °C to 90°C). Comparing to commercial 117 Nafion membrane, all the composite membranes showed an improved performance, and the Nafion-20% In<sub>0.1</sub>Sn<sub>0.9</sub>P<sub>2</sub>O<sub>7</sub> composite membrane is the best in the 10% and 20% and 30% In<sub>0.1</sub>Sn<sub>0.9</sub>P<sub>2</sub>O<sub>7</sub>-Nafion composite membranes. The enhanced DMFC performance might be attributed to the blocking effect of composite membrane for methanol and a high proton conductivity of the composite membrane induced by the "composite effect" between In<sub>0.1</sub>Sn<sub>0.9</sub>P<sub>2</sub>O<sub>7</sub> and Nafion.

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### REINFORCEMENT EFFECT OF SYNTHESIZED ANISOTROPIC SILICA NANOPARTICLES IN INJECTION MOLDED POLYMER COMPOSITES

J. Brent Fox  
Chemical Engineering  
Faculty Research Advisor: Dr. Holly Stretz  
Collaborator: Vijay T. John (Tulane University)

Self-assembled surfactant microstructures can be used as templates to produce inorganic fillers using the principles of colloid and surface science. In this case, mesoporous silica nanowires were synthesized by the Tulane University group [1-2], and "pure" silica nanowires were then incorporated into a composite with nylon-6 using melt compounding techniques. The advantage of these synthesized anisotropic silica nanowires over traditional nanoparticles is that these native nanoparticles tend to be contaminated with trace quantities of Fe and Ti which then cause degradation of the polymer when they are mixed. We presumed that synthetic nanowires would be more compatible with

high temperature polymer processing, and reinforce the polymer without the degradation problems. Here we present modulus data for the composites formed from melt compounding using a DSM 5cm<sup>3</sup> microcompounder and injection molded using a pneumatic-ram type bench scale injection molder.

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### INVESTIGATING NANOPARTICLE DISPERSION IN A MONOMER SOLUTION

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

Composite materials are becoming increasingly important in a number of industries, due to their various advantageous properties, a factor that has led to growing interest in the development of new compounds. The combination of nanoparticles (or nanotubes) and polymers<sup>1</sup> is amongst the most promising of these new materials, but also introduces unique production issues. One of the most troubling of these is the issue of dispersion. Nanoparticles tend to aggregate<sup>2</sup>, and designing a well-mixed system of nanoparticles and polymers is difficult. Experimentally, the level of dispersion is difficult to determine and therefore difficult to alter, but this problem can be avoided by studying the material in silico. By using computer simulations to study systems of nanoparticles and monomers<sup>3</sup> (or varying chain-length polymers), we are able to investigate the factors affecting the dispersion of nanoparticles in the monomer/polymer matrix.

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### MODELING OF ELECTROLYTE CONCENTRATION DISTRIBUTION INSIDE A LITHIUM-ION BATTERY

A. Guduru  
Chemical Engineering  
Faculty Research Advisor: Dr. Venkat Subramanian  
Collaborator: Dr. Vijayasekaran Boovaragavan

In this paper, a novel method of separation of variables developed by Subramanian et al [1] is applied to determine the concentration variations at any point within the various regions of Lithium-ion battery. The closed-form solution obtained using this rigorous mathematical approach can predict the process variations inside the battery more rapidly with accurate solutions. The present work involves the application of the method simultaneously to each region in a full lithium-ion cell i.e. cathode, separator and anode. The solution from this approach is exact and superior to any numerical models currently practiced for the simulation of battery models [2-3]. Also the analytical expressions for concentrations profiles are derived in terms of the relevant system parameters. The system considered for the studies is LiCoO<sub>2</sub>-LiC<sub>6</sub> battery chemistry.

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### SOL-GEL METHOD FOR SYNTHESIS OF LiNi<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub> CATHODE MATERIAL

Jian Hong  
Chemical Engineering  
Faculty Research Advisor: Dr. Chunsheng Wang

The layered LiNi<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub> oxide has become attractive as an alternative cathode material for lithium ion batteries because of its higher capacity, lower cost and enhanced safety features compared to the commercial LiCoO<sub>2</sub> cathode material. However, there are a few drawbacks with the LiNi<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub> cathodes that should be overcome. LiNi<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub> can be considered as a compound among LiNi<sub>0.5-x</sub>Mn<sub>0.5-x</sub>Co<sub>2x</sub>O<sub>2</sub> series. Ohzuku initially prepared it by solid state reaction method and re-prepared by mixed hydroxide method [1]. Chowdari reported that the predominant oxidation states of Ni, Co and Mn in the compound were 2+, 3+ and 4+, respectively [2]. So a closer inspection of their results reveals some contradictory information on the electrochemical behaviors of it. This implied that the electrochemical

characteristics of LiNi<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub> are prone to be affected by preparation condition. In this work, a new sol-gel method was used to prepare the LiNi<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub> cathode materials and their properties were characterized.

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### THERMAL DEGRADATION OF EXPANDED POLYSTYRENE FOAMS

Pravin Kannan  
Chemical Engineering  
Faculty Research Advisor: Dr. Joseph J. Biernacki  
Collaborators: Donald P. Visco Jr. (Chemical Engineering)  
William Lambert (University of Nebraska, Lincoln)

The thermal degradation kinetics of expanded polystyrene foam (sample 1) was studied in various gaseous environments, both oxidizing and non-oxidizing, and in a narrow range of heating rates between 10 and 30 K/min. Kinetic analysis was also performed on monolithic polystyrene films (sample 2) to establish a baseline for comparison. Thermo gravimetric data for both the sample types showed that the mechanism of degradation is different for oxidizing and non-oxidizing conditions. Activation energies of monolithic polystyrene film degradation were found to be in good agreement with literature values. Kinetic parameter values for expanded polystyrene foams have been also reported.

### NANOSIZED Pt/C CATALYSTS SYNTHESIZED BY CONVENTIONAL AND MICROWAVE-IRRADIATED METHODS

Jianxin Ma  
Chemical Engineering  
Center for Manufacturing Research  
Faculty Research Advisor: Dr. Chunsheng Wang

The development of low-temperature fuel cells has been an increasing interest due to their numerous advantages and huge potential application values [1-3]. In this work, a 20wt% Pt/C catalyst was successfully synthesized by a conventional refluxed (CR) heating method and a microwave-irradiated (MI) heating method, respectively. The element composition, phase structure and micro-morphology of the MI Pt/C and CR Pt/C catalysts were determined using SEM/EDX, XRD and TEM, and their electrocatalytic activities to methanol oxidation of the catalysts were evaluated using a conventional three-electrode test cell, and compared with the performance of a commercial E-TEK Pt/C catalyst. The MI Pt/C catalysts have a smaller particle size, more uniform particle distribution, and higher oxide contents on the surface layer of Pt particles than



that of CR Pt/C, which result in a low onset potential, a high current density of MI Pt/C catalysts.

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### ELECTROKINETIC-BASED DRUG DELIVERY THROUGH THE SKIN AND SEPARATION OF BIOMACROMOLECULES

Jennifer Pascal and Ryan O'Hara  
Chemical Engineering  
Faculty Research Advisor: Dr. Pedro Arce  
Collaborator: Mario Oyanader (Chemical Engineering)

Electrokinetic-based methods are a promising way to accomplish effective and non-invasive delivery of drugs. By using a capillary model for the skin and, applying the principles of electrostatics and hydrodynamics, velocity profiles were determined for two types of idealized capillary geometries assumed to exist in the skin, rectangular and cylindrical. Volumetric flowrates were determined for both geometries so that effect of the geometry in predictions can be assessed. Electrokinetic-based methods are also useful in Bio-Separations. It has been found that applying an electrical field orthogonally to a Poiseuille flow regime, decreases the optimal separation time [1]. Therefore, a similar analysis was performed for a Couette-electrokinetic based separator, often used to separate biomacromolecules. By utilizing the area averaging technique along with the principles of electrostatics and hydrodynamics, effective parameters were determined to predict optimal times of the separation of biomacromolecules.

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### DEVELOPING EFFICIENT MODELS FOR THE CONTROL OF FUEL CELLS

Robert Phillips and Vinten Diwakar  
Chemical Engineering  
Faculty Research Advisor: Dr. Venkat Subramanian

Mathematical models for fuel cells in hybrid environments involve the solution of coupled non-linear partial differential equations that describe current, voltage, and concentrations of electrochemical species as functions of time and position throughout the system [1-2]. The solution to these models

requires high computing capability which creates a big cost. When the model is used to optimize the design of the fuel cell, it further increases the cost. This poster presents a simplification method used on rigorous model of pressure[3] and concentration in a fuel cell.

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### EFFECT OF PURE COMPONENT PARAMETERIZATION METHODOLOGY ON MIXTURE PROPERTY PREDICTIONS FOR THERMODYNAMIC EQUATIONS OF STATE USING TERRAIN METHODOLOGY

Saravanan Swaminathan  
Chemical Engineering  
Faculty Research Advisor: Dr. Donald P. Visco, Jr.  
Collaborator: Angelo Lucia (University of Rhode Island, Kingston)

This research focuses on studying the predictive power of a complex thermodynamic equation of state (here, SAFT-VR EOS) that will, in turn, improve one's ability to model complex systems in the future. This work attempts to characterize and maximize the predictive ability of the model by mitigating spurious conclusions that are based on results from local minimization schemes. Thus, allowing for more definitive conclusions on the properties of systems in the absence of experimental data. To this end, this work employs global terrain methodology [1] – an advanced global optimization technique and applies it to the field of thermodynamic modeling. Additionally, analyses on the effects of multiple parameter-sets and binary interaction parameters on the prediction of mixture properties will be discussed. Through this work, parameter rules will be developed that will allow for the optimal prediction of pure component properties.

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### EXPERIMENTAL ASSESSMENT OF BUOYANCY DRIVEN FLOWS IN AN ELECTROKINETIC (EK) CELL FOR SOIL REMEDIATION

Cynthia Torres - Godoy  
Chemical Engineering  
Faculty Research Advisors: Dr. Pedro Arce and Dr. Mario Oyanader

EK soil remediation has been identified as a versatile technology to remove heavy metals and hydrocarbons from a contaminated site. Although temperature development on the soil matrix has been observed, little effort has been dedicated to use temperature-triggered mechanisms as potential advantages rather than pitfalls. A simple statistical analysis has been performed on the experimental data to determine whether there exist an effect of buoyancy driven flows on the over all removal efficiency. Kaolin based soil media previously spiked with different contaminants was used in the experimental runs. The EK cell was placed at different inclined positions to verify the influence of buoyancy driven flows on the efficiency of contaminant removal. The results and conclusions derived from this study are the baseline for the EK cell system modeling. Comprehensive details of key factors are highlighted to illustrate the modeling technique as well as the system behavior.

### APPLICATIONS OF SIGNATURE FOR MOLECULAR DESIGN

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

Quantitative structure-activity relationships (QSARs) are models which utilize descriptors to relate the structure of a compound to a specific molecular property of interest. Plugging in the values of descriptors for a given compound into the QSAR will give a prediction of the property for that compound. This process is recognized as the forward QSAR problem. [1] QSARs can be employed to refine the search for molecules matching a desired property in an existing database, but ideally one would like to examine potential compounds outside the database. Here we present a novel algorithm to accomplish that goal, which involves solving the inverse-QSAR (I-QSAR) problem via a powerful molecular descriptor known as Signature. [2] Diophantine constraint equations are generated based on valence and consistency restrictions to solve the inverse problem. In our previous work with hydrofluoroethers (HFEs) [3], the size of the compounds in the database was relatively small (10-30 atoms) and the inverse problem was easily solved. For larger compounds (50-100 atoms), the number and complexity of the constraint equations increases greatly which makes solving them challenging.

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### COMPARISON OF PREPARATION TECHNIQUES OF IRON SILICIDE ELECTRODES IN LITHIUM ION BATTERIES

Shannon Wroblewski and Jian Hong  
Chemical Engineering  
Faculty Research Advisor: Dr. Chunsheng Wang  
Collaborator: Dr. Jianxin Ma (Chemical Engineering)

Iron silicide (FeSi75) was used as the primary anode material in a Li-ion cell in which different preparation techniques were compared. Techniques such as milling/mixing method, rolling of the electrode sheet, heat treatment of the electrode material, alteration of the slurry ratio, and graphite alterations were all compared based on cycle life and irreversible capacity. Iron silicide that was ball milled with graphite for fifteen minutes and was then heat treated under a nitrogen atmosphere yielded some of the best results. Its reversible capacity was approximately 375 mAh/g and was stable for nearly 50 cycles.

### EXPERIMENT AND MODELING OF POLYOL+BLOWING AGENT MIXTURES

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

This research focuses on evaluating the correlative ability of thermodynamic models like Sanchez-Lacombe EOS to describe polyol-blowing agent systems using the experimental solubility data for different polyol + blowing agent combinations. As very limited experimental solubility data of environmental-friendly (non-ozone depleting) blowing agents in polyols is available, an experimental setup is being designed to obtain this data. The process includes designing of a degassed vapor pressure apparatus [1] to run the experiments for some of the polyol + blowing agent combinations. After obtaining the experimental data we



will use this data to determine the predictive ability of the SL equation of state with the help of a binary interaction parameter.

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## CHEMICAL ENGINEERING UNDERGRADUATE STUDENTS

### DIFFUSION OF GAS IN POLYSTYRENE FILMS

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

Surprisingly little is known about diffusion of even common gases in polystyrene (PS). The rate of transfer of blowing agents, for example, and the effect of gas exchange in expanded PS foam depends on reliable prediction of diffusion through the bulk medium and its foamed counterparts. A simple diffusion apparatus was designed and experiments were conducted to provide data on gas diffusion in solid films. The data was fit to a numerical model and a computer simulation was developed to take data from film experiments and predict how gases diffuse through the microstructure of PS foam. Diffusion coefficient values of argon molecules through PS are presented and the effect of film thickness on mass flux has also been reported.

### INVESTIGATING TUMOR GROWTH IN THE PRESENCE OF DRUGS

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

Cells continuously adapt to changing conditions through coordinated molecular and mechanical responses. As cells evolve for their surroundings, uncontrollable, abnormal growth patterns can occur leading to cancer. These events can be studied using different methodologies. Mathematical models can integrate the different aspects of complex tumor growth allowing for a non-experimental study of cancer.[1-3] We use the cellular automaton model to take into account multiple factors affecting tumor growth in tissue. In this in silico "experiment," a multiscale mathematical model of tumor growth based upon molecular and life cycle features is used. This model includes life cycle parameters such as replication rate and life span and possible drug effects. This type of model can be used to test prototype drugs and compare their effectiveness on tumor growth under

different conditions and location of application.

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### THE EFFECT OF CHARGED LAPONITE NANOPARTICLES ON POLYACRYLAMIDE ELECTROPHORESIS OF PROTEINS

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

Currently, there is an interest in novel drug delivery systems and diagnostic capabilities. One possible approach is to add charged nanoparticles to the polyacrylamide gel electrophoresis system to observe the difference in protein separation efficiency. Another approach included creating templated pores by polymerizing a polyacrylamide gel with various macromolecules (including DNA, xanthan, and SDS) randomly dispersed throughout the gel and removed before performing gel electrophoresis, which improved protein separation efficiency<sup>1</sup>. Polyacrylamide gels were successfully cast and crosslinked with well dispersed, charged nanoparticles of varying diameters (Southern Clay Laponite RD and an experimental Laponite) at a concentration of approximately 1% (w/w). The nanoparticle dispersion is characterized by the visual clarity of the resultant gels and by environmental scanning electron microscopy. The charged nature of the nanoparticles is expected to improve the protein separation efficiency of the polyacrylamide gel, by comparison to the analogous system where templated pores were introduced into the gel. Future work could include modifying the current drug delivery systems to optimize the performance capabilities of pharmaceuticals.

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## CHEMICAL ENGINEERING POST-DOCTORAL FELLOWS

### A NEW APPROACH FOR RAPID INITIALIZATION OF BATTERY MODELS

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

Secondary batteries are usually modeled as a system of coupled nonlinear partial differential equations [1]. These models are typically solved by applying finite differences or other discretization techniques in the spatial directions and solving the resulting system of differential algebraic equations (DAEs) numerically in time. These DAEs are very difficult to solve even using popular DAE solvers [2] due to initialization problem. In this work, a shooting method is proposed as an effective and rapid technique for the initialization of battery models. Notably, the computation time required for the proposed method is only milliseconds in a FORTRAN environment for the case of initializing a standard physics based lithium-ion battery model. Also the initial values obtained are exact and can readily be fed into any DAE solver for achieving accurate solutions without solver failure.

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### A NOVEL SIMULATION METHODOLOGY FOR COPPER DEPOSITION

Harini Seshadiri  
Chemical Engineering  
Faculty Research Advisor: Dr. Venkat Subramanian

A novel simulation methodology is developed which incorporates the ionic and molecular sizes for estimating the free energy of activation involved in the deposition of copper. The number of molecules including the solvent (water in the present case) is 22592 (18000 water molecules). The simulation box size assumed is 354Å. As an initial step the free energy of activation obtained from the present methodology agrees satisfactorily with literature. This methodology needs further refinement to understand the exact chemistry behind the process of copper deposition in the presence of additives.

## CIVIL AND ENVIRONMENTAL ENGINEERING GRADUATE STUDENTS

### INTERNAL CURING MATERIALS TO MITIGATE EARLY AGE SHRINKAGE IN HIGH PERFORMANCE PORTLAND CEMENT MORTARS

Kristen Batey  
Civil and Environmental Engineering  
Faculty Research Advisor: Dr. Benjamin Mohr

With the advent of high performance concrete containing low water-to-cement ratios, early age shrinkage cracking of concrete has occurred with greater frequency. Early age cracking (primarily due to autogenous shrinkage) significantly compromises the durability of the concrete. This research program is investigating the effect of internal curing materials such as saturated lightweight aggregates on cement pastes, mortars, and concretes. Currently, internal curing materials have been evaluated for their shrinkage reducing effectiveness in cement pastes and mortars at early and later ages. One important aspect of this research will be to investigate the movement of internal curing water in the cementitious microstructure at early ages. Analytical techniques are presently being considered to assess the distance and rate of water transport through the microstructure. The ability to determine an effective area of influence around internal curing materials would significantly improve the understanding of water movement through the evolving pore structure.

### DEVELOPMENT OF AN OPEN-BOOK WATERSHED

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

Proposed NASA mission, Global Precipitation Measurement (GPM) may now usher a new era of application of the open-book modeling framework to understand the applicability of high resolution satellite rainfall data for predicting transboundary river flow. We developed, verified and implemented our open-book watershed model for rapid prototyping of satellite rainfall based flood monitoring systems for International River Basins (IRBs). We simulate the stream-flow hydrograph using radar (WSR-88D) rainfall data over Oklahoma assuming an open-book configuration. Using the radar-simulated hydrograph as the benchmark, and assuming a two-nation hypothetical IRB over Oklahoma, we explored the impact of assimilating NASA's real-time satellite rainfall data (IR-3B41RT) over the upstream nation on the flow monitoring accuracy of the downstream nation. We developed a relationship defining the improvement in

flow monitoring that can be expected from assimilating IR-3B41RT over transboundary regions as a function of the relative area occupied by the downstream nation.

### ERROR BUDGET ANALYSIS OF HYDROLOGIC MODELS USING SATELLITE RAINFALL DATA

Preethi Raj  
Civil & Environmental Engineering  
Faculty Research Advisor: Dr. Faisal Hossain

In the absence of an adequate ground-based rainfall network, satellite-based rainfall estimates become the natural alternative which is prone to errors. We hypothesize that error in rainfall is a conservable quantity for hydrologic models that honor the principle of conservation of mass and should be amenable to closure through tracking of the distribution of the input error from rainfall to the various hydrologic stores/fluxes/components that are predicted. In this study, we conduct an analysis of progression of error from the input stage to various components simulated by the model to identify the level to which the assumption of the conservation of error can be validated. We propose to conduct error budget analyses using four hydrologic models. Our goal is identify the relative proportion of accumulation of error in the various variables that are predicted by the model as a function of rainfall error type, space-time scales as well model complexity.

### EFFECT OF SKEWNESS ON LIVE LOAD REACTION AT PIERS OF CONTINUOUS BRIDGES

Qinghe Zhang  
Civil and Environmental Engineering  
Faculty Research Advisor: Dr. X. Sharon Huo

In the AASHTO LRFD Specification [1], the skew correction factors for beam are used to take into account the effect of bridge skewness on moment and shear distribution factors in skewed bridges. It has been observed in some studies [2, 3] that the reactions at piers in a skewed continuous bridge are amplified and the skew correction factors for reactions are unique from those for beam shear. This project investigates the effect of bridge skewness on live load reactions at piers of continuous skewed bridges with finite element analyses. The comparison of the distribution factors of live load reactions and shear revealed that the distribution factor of reaction at piers was higher than that of shear at beam ends near the same support. The increase in reaction distribution factor was more significant than that in shear distribution factor on the interior beam line when skew angle was greater than 30°. The LRFD shear equations and the Lever Rule method could conservatively predict live load reaction distribution for piers on exterior beam lines but underestimate live load reaction on interior beam lines.

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### DISTRIBUTION FACTORS OF LIVE LOAD MOMENT FOR STEEL OPEN BOX GIRDER BRIDGES

Lei Zheng  
Civil and Environmental Engineering  
Faculty Research Advisor: Dr. X. Sharon Huo

Bridge design engineers have utilized the concept of distribution factors to evaluate the transverse effect of live loads since the 1930s.[1] The current AASHTO LRFD[2] equation of live load moment for steel open box girder bridges has not been updated for more than 40 years. Modern bridges have longer span length, higher material strength, smaller cross section, and heavier loads than bridges decades ago. Bridge community has urgent needs to investigate the availability of distribution factor for open box-girder bridges. In this study, finite element analysis method will be performed to obtain the distribution factors of live load moment for steel open box girder bridges. The distribution factors from the AASHTO LRFD equations will be compared to that obtained from the analysis. The comparison will review the shortcomings of current AASHTO LRFD and suggestions will be given on the modification of live load distribution factor equations.

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## ELECTRICAL AND COMPUTER ENGINEERING GRADUATE STUDENTS

### AN OVERVIEW OF VIRTUALIZATION TECHNOLOGY

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

As modern computers grow more powerful, virtualization technology begins to regain attention in both industry and academic areas [1]. Numerous systems have been built with virtualization technology to extract the underlying hardware resource of the computers. However there are still many challenges that virtualization specialists should face: the isolation of different virtual machines (VM); the support for commodity operating systems and applications; and the performance overhead [2]. Various virtualization technologies have been adopted to fulfill the promised performance. This paper conducts a survey of virtualization technology and then focuses on storage virtualization [3]. We present how to design, implement and evaluate a storage virtualization.

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3. Tom Clark. Storage Virtualization : Technologies for Simplifying Data Storage and Management. Addison-Wesley. March 2005.

### LU DECOMPOSITION ON MATLAB DISTRIBUTED COMPUTING

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

In the field of engineering, many systems are built on a physical model with linear relationship. With the increase of the dimension of a problem such as  $Ax = b$ , the problem size grows dramatically. LU decomposition method can help reduce the problem size. However, the size of problem still grows cubic as the dimension grows, therefore the time required to solve such a problem is very long. Our objective is to reduce the computation time by using Matlab DCT (Distributed Computing Toolbox). The work has been done with 3 desktops PCs. One of the 3 desktops served as

headnode running 3 workers, while the other 2 desktops run 1 worker each. The results show that with large problem size, 1000-by-1000 matrix for example, the speedup (Sequential Execution Time divided by Parallel Execution Time) is approximately 4.8.

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### L2 CACHE EVALUATION OF MULTICORE ARCHITECTURES

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

Due to the physical limitations such as power usage and heat dissipation to the current processor design, the industry is turning to multicore processor design from uniprocessor. Currently, several vendors like Intel, AMD, IBM, and Sun have delivered their own multicore processors to the market. However, the cache performance for various multicore processor architectures is not fully exploited. The cache performance, especially L2 cache, is a function of cache architectures (shared or private), cache organizations (direct mapped, fully associative or set associative), the cache replacement policy (FIFO, LRU, LFU, Random, or MRU), and cache capacity. This paper presents a comprehensive performance evaluation on L2 cache based on Intel Core 2 and AMD Athlon multicore architectures using the cycle-accurate simulator SESC.

### DESIGN AND IMPLEMENTATION OF A CONTROL SYSTEM FOR A COUNTER GRAVITY CASTING MACHINE

W. A. Deabes and M. Davis  
Electrical and Computer Engineering  
Faculty Research Advisor: Dr. Mohamed Abdelrahman

In counter-gravity casting [1], pressure is used to draw molten metal, against gravity, into the flask in order to replace the foam pattern and form the final product. The performance of the current pressure controller needs improvement to increase the quality and repeatability



of the final product. There are two major hardware difficulties that needed to be compensated for. The first is the nonlinear behavior of valves (Hysteresis Nonlinearity), which is addressed using a gain scheduling approach by decomposing the nonlinear system into approximate linear sub-systems. Consequently, each linear sub-system is controlled using a PID controller [2, 3]. The second difficulty is the decrease of the plenum pressure responsible for creating the vacuum, which requires a new control approach. A PID controller with a gain scheduling scheme [4, 5] and a feed forward term was developed to overcome the nonlinear characteristic [6] of the valves and to compensate for variation of the pressure inside the plenum. The new controller showed considerable performance improvements. Furthermore, the experimental results show how the control is robust in the presence of significant dynamic variations in the input profile.

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#### INTER-DOMAIN ROUTING IN DWDM NETWORKS

Qing Liu and Mehmet Ata Kök  
Electrical and Computer Engineering  
Faculty Research Advisor: Dr. Nasir Ghani

Dense wavelength division multiplexing (DWDM) [1] has become the dominant transport layer technology for next-generation backbone networks due to its unprecedented capacity scalability. As a result, there is a pressing need to investigate lightpath provisioning in multi-domain DWDM networks [2]. Although inter-domain provisioning has been well-studied for packet/cell-switching networks, the wavelength dimension (along with wavelength conversion) presents many added challenges. To address these concerns, a detailed GMPLS-based hierarchical routing framework for provisioning transparent/translucent/opaque multi-domain DWDM networks is presented. The scheme adapts topology abstraction to hide internal domain state so as to resolve routing scalability and security issues. Specifically a novel full-mesh topology abstraction scheme is developed for full wavelength conversion domains, i.e., to disseminate additional wavelength converter state. Related inter-domain lightpath RWA [3] and signaling schemes

are also tabled. Performance analysis results are then presented to demonstrate the effectiveness of the proposed mechanisms along with directions for future research work.

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#### DETERMINATION OF FEEDER LOSSES BY AN IMPROVED LINEAR MODEL IN A RADIAL CIRCUIT

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

Feeder losses play an important role in the economics of a distribution system. In the traditional power flow analysis algorithms, the losses are determined as a follow up of the feeder voltages and currents. In this paper the line flow based analysis proposed by Yan and Sekar [1] is extended to derive an improved linear model that can directly evaluate the losses with sufficiently good accuracy. The proposed technique uses feeder section power and reactive power and the receiving end voltage as the variables to be determined. After writing line voltage equations and power and reactive power balance equations at each feeder section, the improved linear model is derived using the Taylor series expansion.

The improved model is applied to the standard IEEE 13 Node Test Feeder distribution system and shown to provide the losses quite accurately. The paper provides extensions of application of the model to solve some practical problems.

#### COMPACT MODELING ON NANOSCALE CMOS DEVICES

Sudheer Vootkuri  
Electrical and Computer Engineering  
Faculty Research Advisor: Dr. Stephen Parke

The ITRS roadmap projects that double-gated transistors will be needed in the future, in order to scale CMOS to the 32 nm node. Flexible dynamic threshold control is possible with independently- double gated (IDG) CMOS technologies, and is highly desirable for ultra-low-power (ULP) SoC designs. By varying the bottom gate voltage of the FlexFET IDG MOSFET from -0.5V to +0.5V, standby power can be dynamically changed over ten orders of magnitude, while the transistor/

circuit performance can be changed by 70%. Minimally sized transistors may be used to achieve ULP in the standby, while dynamic Vt adjustment is used to achieve high performance when active. This poster demonstrates IDG Flexfet CMOS transistor, their dynamic threshold model and compact models that incorporate these effects. IDG-CMOS has also been recently applied to several exciting new analog/MS/RF circuit applications.

#### EVALUATION OF A SCALAR MULTIPLY-ACCUMULATE DESIGN WITH FAST MULTIPLIER

Sara Woods  
Electrical and Computer Engineering  
Faculty Research Advisor: Dr. Roger Haggard

This research in computer arithmetic architectures evaluates the implementation of 8, 16, and 32-bit multiply-accumulate units using the Kang-Gaudiot multiplier presented in

1. The Kang-Gaudiot multiplier implements a fast two's complement conversion of the last partial product term to reduce delay in the multiplier by one stage. The general multiply-accumulate unit is similar to the Fadavi-Ardekani
2. style Booth encoded multiplier with a carry-lookahead adder [3] for the accumulator. The three versions of both architectures are compared in synthesis size, multiply accumulate rates, and maximum frequency. Simulation and synthesis is performed using Mentor Graphics' ModelSim and Altera Quartus II with a target device of the Altera Cyclone II EP2C35F672C6 FPGA.

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#### TIME REVERSAL FOR UWB COMMUNICATIONS

Chenming Zhou and Qiang Zhang  
Electrical and Computer Engineering  
Faculty Research Advisor: Dr. Robert Qiu

This paper experimentally investigates the scheme of time reversal (TR) combined with multiple-input single-output (MISO) antennas over ultra-wideband (UWB) channels. In particular, temporal and spatial focusing as well as array gain are studied based on a 4\*1 MISO scheme in an office environment.

The results confirm that the energy of UWB signals in an

MISO scheme is more spatial-temporally focused than in a single-input single-output (SISO) scheme. As a result, a strong peak is observed in the equivalent channel impulse response. The magnitude of this peak grows linearly with the square root of the number of antenna elements at the transmitter. All the measurements and data processing are completed in the time domain.

Based on the experiment results, a UWB testbed with TR capability is developing in our lab. Some of the most recent results on the testbed will be shown.

### ELECTRICAL AND COMPUTER ENGINEERING UNDERGRADUATE STUDENTS

#### SYSTEM IDENTIFICATION AND CONTROL OF COUNTER GRAVITY SYSTEMS

Malik Davis  
Electrical and Computer Engineering  
Faculty Research Advisor: Dr. Sally Pardue (Mechanical Engineering)

The research performed was used to develop a controller for a counter gravity casting machine. The counter gravity casting machine was originally a SISO system that uses a transducer to turn voltage into a pressure that is used to control the position of two valves. This setup uses a PID controller to control the voltage that is being sent to the transducer and thus controls the pressure in the system.

While this setup has the advantage of being very simple, it tends to respond poorly within certain pressure ranges. This poor response is attributed to the pressure in the plenum that dramatically decreases during periods of high flow rate through the valves. After this period of high flow rate the system struggles to reach pressures any higher than its current state. The research done describes different methods and controllers that avoid the problem with high flow rate.

### INDUSTRIAL AND SYSTEMS ENGINEERING UNDERGRADUATE STUDENTS

#### PARAMETER UTILIZATION IN THE CROSS DOCK PROBLEM

Chad Bournes, Jennifer Cloud, Vanessa Kasten, Jake Mitchell, Chris Potts and Tarrah Wilkerson  
Industrial and Systems Engineering  
Faculty Research Advisor: Dr. David Elizandro

In the cross dock environment arriving freight, measured in handling units, are moved from a trailer to a stripping door to a destination trailer at a loading door (Elizandro). The



goal in the cross dock problem was to find the most efficient layout of shipping and receiving doors, subject to material and distance constraints. This representation of the cross dock problem is an application of the quadratic assignment problem (Taha). A genetic algorithm was created to search for the five best configurations. The algorithm incorporates set parameters, e.g., number of chromosomes, mutations, and gene splices, that affect the performance of the search (Cheng). This research study will identify which algorithm parameters have the greatest affect on finding the best solutions in the least amount of time.

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## MANUFACTURING AND INDUSTRIAL TECHNOLOGY UNDERGRADUATE STUDENTS

### ANALYSIS OF LOST FOAM CASTING GRAIN REFINEMENT IN MAGNEIUM AM60B

James Droke  
Manufacturing and Industrial Technology  
Center for Manufacturing Research  
Faculty Research Advisor: Dr. Kenneth Currie  
Collaborator: Qingyou Han (Oak Ridge National Laboratory)

The addition of hexachloroethane aides as a degas agent and a means of grain refinement when added to cast metals. By using a vacuum chamber and a 1% solution of hexachloroethane dissolved in ethanol, the foam was impregnated with a small amount of the degas agent. Thirty six samples were analyzed with the use of a microscope and austenite reticle after a two hour heat treatment followed by mounting, grinding, polishing and etching all samples. Through a series of experiments including different types of foam, the addition of hexachloroethane through impregnation, addition of degas agent in molten metal and without degas agent was tested and analyzed. The results show that the addition of hexachloroethane inside the pattern before casting is better in reducing grain size than no degas agent. Using the degas agent in the molten metal with a low fusion level foam resulted the lowest average grain size.

## MECHANICAL ENGINEERING GRADUATE STUDENTS

### FATIGUE FAILURE THEORY FOR COMPLIANT MECHANISM DESIGN

Justin Helton  
Mechanical Engineering  
Faculty Research Advisors: Dr. Joseph Richardson and Dr. Stephen Canfield

Compliant mechanisms (CMs) are single-part devices that achieve desired force and displacement characteristics through elastic deformation of their structure. Buckingham Pi terms are developed to characterize the fatigue behavior of arbitrary single input single output compliant mechanisms. These Pi terms will be validated using experimental data collected on multiple configurations of compliant mechanisms using the same input and output conditions. This presentation will discuss TTU's current multi-objective optimization genetic algorithm code and activities to improve fatigue behavior predictions.

### CFD MODELING OF RESIDENCE TIME IMPROVEMENT IN AN INDUSTRIAL BOILER

Murthy Lakshmiraju  
Mechanical Engineering  
Faculty Research Advisor: Dr. Jie Cui

The overall combustion efficiency of a grate fired furnace in an industrial boiler depends on the mixing of the secondary air with the off-bed gases. Previous research has established residence time of the under grate air in the boiler as a critical parameter that affects the combustion. This project discusses the state of the art of techniques used in industrial boilers to improve the residence time: Ecotubes and Ecojets. Ecojet is a relatively newer technique over the Ecotube system that distributes the secondary air more evenly and effectively. The main objective of this project is to increase the flow residence time of the under grate air by replacing the Ecotube air system with the Ecojets. This project presents the cold flow simulation results using Fluent and discusses the mechanism of the residence time increase. The optimum location of the Ecojets and the injection angle were identified for a typical 36MW boiler and a 20% increase in residence time was attained.

### MODELING FRICTION STIR WELDING HEAT TRANSFER

Satish Perivilli  
Mechanical Engineering  
Faculty Research Advisors: Dr. John Peddieson and Dr. Jie Cui

Friction Stir Welding (FSW) heat transfer has been an area of concentrated research over the past few years [1-5]. The amount of heat generated during the process defines the quality of weld, its mechanical properties and workpiece and tool distortion. For this study, a quasi-steady numerical model pertinent to a typical partial penetration configuration is developed using FLUENT and validated with its literature source. Subsequently, this formulation is extended to full penetration and self-reacting FSW configurations. Mechanical dissipation heating, responsible for the welding is modeled by means of a thermal boundary condition at the tool surfaces. The resulting temperature distributions are analyzed at various planes and lines for the three configurations studied. It is shown that the partial and full penetration models predict the same peak temperature whereas the self-reacting configuration predicts a higher temperature owing to the additional bottom shoulder.

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### GENERAL MOBILITY IDENTIFICATION AND RECTIFICATION OF WATT AND STEPHENSON SIX-BAR LINKAGES

Jun Wang and Changyu Xue  
Mechanical Engineering  
Faculty Research Advisor: Dr. Kwun-Lon Ting

Mobility identification is a common problem encountered in linkage analysis and synthesis. Mobility of Watt as well as Stephenson six-bar linkages refers to the problems related to branch defect, full rotatability, singularities, and order of motion. For Watt six-bar linkages, the answers to these problems had been restricted to special conditions requiring the input be placed in the common link shared by two four-bar chains. For Stephenson six-bar linkages, the input

and output joints were required to be placed in the same four-bar loop. This paper offers a unified and comprehensive treatment for any input and output conditions. It presents answers to all typical mobility issues, offers the geometric insight as well as explanation on the effects of multiple loops to any intended output or functional relationship, and hence casts light for treating other complex linkages. Besides, an idea of scaling and rotating is offered to simplify the original Watt six-bar linkage. Several examples are employed to demonstrate the method in all input and output conditions.

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## MECHANICAL ENGINEERING UNDERGRADUATE STUDENTS

### MODIFIED TRICYCLE FOR HANDICAPPED CHILD

Raymond Allan Bowker  
Mechanical Engineering  
Faculty Research Advisor: Dr. Stephen Canfield

Dr. Stephen Canfield presented the team of student engineers with a need for a tricycle for a child that has very

limited use of his lower body. The team asserted that the child would need to be able to power the tricycle with his upper body. A proposed solution was to redesign an existing tricycle to be powered by "pumping" the handle bars back and forth. The problem the team faced with this solution was that if the tricycle were pushed or rolling down a hill, the handle bars could become a hazard to the child. Another proposition arose to use a unidirectional bearing that would only allow the handle bars to crank the wheel and not vice versa. This caused the team to face another problem to the effect that the wheel would only crank for pushing the bars forward or backward, but not in both conditions. The team researched a design to crank the wheel over the toggle positions and allow it to crank with forward and backward pumping of the handle bars.

## ULTRASONIC EVALUATION OF THE FUSION LEVEL OF EXPANDED POLYSTYRENE FOAM

James Klein  
Mechanical Engineering  
Faculty Research Advisor: Dr. Sally Pardue

The quality of the metal parts produced using the lost foam casting (LFC) process has been shown to be a function of the properties of the expanded polystyrene (EPS) foam used in the process. As much as 90% of the problems associated with the LFC industry are believed to be direct results of problems with the foam used.

An important EPS foam property is its fusion level. This is a measure of how well the polymer chains have intertwined

and / or joined at the bead to bead boundaries. Research has shown that fusion level does have a strong effect on mold fill times and thus an effect on the quality of the metal cast.

For the purposes of this research, a thru-transmission, low frequency, ultrasonic testing technique was and is being used. A correlation between fusion level and ultrasonic velocity in the foam is trying to be established.

## NONDESTRUCTIVE INFRARED THERMOGRAPHY FOR CHARACTERIZATION OF EPS FOAM FUSION

Viktor L. Orekhov  
Mechanical Engineering  
Faculty Research Advisor: Dr. Sally Pardue

The degree of fusion in foam patterns has been shown to have a significant effect on defects in the lost foam casting process. As a result, an increasing amount of interest has developed to find a method capable of measuring fusion nondestructively. In the present research, several infrared techniques typically used in thermography have been examined in an effort to develop a method of characterizing bead fusion. The results indicate that one-sided techniques will be challenging to implement due to the foam properties in the infrared spectrum. Nevertheless, a two-sided technique has been developed which exploits infrared radiation to reveal fusion variations within a pattern. The technique has been effectively used in both qualitative and quantitative measurements on simple patterns.

## ACKNOWLEDGEMENTS

The Research Day Committee gratefully acknowledges everyone who contributed in any way to the success of Student Research Day 2007. 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 67 abstracts involving ~80 undergraduate and graduate students, more than 30 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 and to James Mabery for 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.

The awards that will be provided for the best posters were designed and manufactured as part of a senior research project by students in Dr. Ahmed ElSawy's Manufacturing and Industrial Technology class.

It was a pleasure working with Dr. ElSawy and these students on this project, and we are extremely grateful to them for the significant contributions that they all made.

We would also like to thank President Bell and Provost Barker for their continued support of this program. 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, 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. Sue Bailey  
Dr. Subramaniam Deivanayagam  
Dr. Wade Faw  
Dr. Virginia Moore  
Dr. Shelia Green  
Dr. Paul Semmes  
Dr. John Wheeler  
Dr. Robby Sanders  
Dr. Francis Otuonye

## COLLEGE OF ARTS AND SCIENCES

Michael Baldwin .....	6
Wesley Bland .....	8
Samuel Bledsoe .....	8
David Wayne Cook II .....	10
N.W.S.V. Nuwan DeSilva .....	6
Jeremy Ey .....	7
Robby Florence .....	8
Kyle Guillot .....	8
Matt Hermanson .....	9
Chandra Sekhar Jamalpur .....	7
Brandon Malone .....	7
Viatcheslav Meisner .....	9
Stan Paulauskas .....	11
Derek Pennycuff .....	9
David Priebel .....	10
Michael Rohling .....	9
Jun Tokiwa .....	11
Andrew Walker .....	7
Robert Wilkinson III .....	10

## COLLEGE OF EDUCATION

Xiuchang Ann Huang .....	12
--------------------------	----

## COLLEGE OF ENGINEERING-CHEMICAL

Barath Baburao .....	13
Prasad Bhosale .....	13
Jennifer Bollig .....	18
Vijayasekaran Boovaragavan .....	19
Vinten Diwakar .....	13, 16
Bin Fang .....	14
James Brent Fox .....	14
Deepika Gollamandala .....	14
Anupama Guduru .....	15
Jian Hong .....	14, 15, 17
Pravin Kannan .....	15, 18
David Kirby .....	18
Jianxin Ma .....	15
Ryan O'Hara .....	16
Jennifer Pascal .....	16
Robert Phillips .....	16
Nemoy Rau .....	18
Hope Sedrick .....	18
Harini Seshadiri .....	19
Saravanan Swaminathan .....	16
Cynthia Torres-Godoy .....	17
Derick Weis .....	17
Shannon Wroblewski .....	17
Satya Suresh Yelisetty .....	17

## COLLEGE OF ENGINEERING-CML AND ENVIRONMENTAL

Kristen Batey .....	19
Nitin Katiyar .....	19
Preethi Raj .....	20
Qinghe Zhang .....	20
Lei Zheng .....	20

## COLLEGE OF ENGINEERING-ELECTRICAL AND COMPUTER

Peng Chen .....	21
Xi Chen .....	21
Xin Chen .....	21
Malik Davis .....	21, 23
Wael Deabes .....	21
Qing Liu .....	22
Mehmet Ata Kök .....	22
Ndaga Mwakabuta .....	22
Sudheer Vootkuri .....	22
Sara Woods .....	23
Chenming Zhou .....	23
Qiang Zhang .....	23

## COLLEGE OF ENGINEERING - INDUSTRIAL AND SYSTEMS ENGINEERING

Chad Bournes .....	23, 24
Jennifer Cloud .....	23, 24
Vanessa Kasten .....	23, 24
Jake Mitchell .....	23, 24
Chris Potts .....	23, 24
Tarah Wilkerson .....	23, 24

## COLLEGE OF ENGINEERING - MANUFACTURING AND INDUSTRIAL TECHNOLOGY

James Droke .....	24
-------------------	----

## COLLEGE OF ENGINEERING - MECHANICAL

Raymond Allan Bowker .....	25, 26
Justin Helton .....	24
James Klein .....	26
Murthy Lakshmiraju .....	24
Viktor Orekhov .....	26
Satish Perivilli .....	24, 25
Jun Wang .....	25
Changyu Xue .....	25

# NOTES AND COMMENTS



