Georgia Tech Institute of Paper Science and Technology

2011 Executive Conference
Student Poster Session

The following are abstracts of the research work currently being conducted by a sampling of the Paper Science and Engineering graduate students. Funding for these students is largely provided by the industry-generated endowment fund. The students are members of a multi-disciplinary education and research program for the pulp and paper industry and are pursuing degrees through the mechanical engineering, chemical and biomolecular engineering, materials science and engineering, and the chemistry & biochemistry schools of the Georgia Institute of Technology.

Electrochemical Treatment of Flexographic Wastewater
Author: Alexander T. Jordan
Email: atjordan@gatech.edu
Advisor: Dr. Jeffery S. Hsieh
Abstract: Flexographic ink filtrate was treated using electro-flocculation. Decontamination efficiency was determined with turbidity and cationic demand. A model flexographic ink concentration of 0.044 mg/mL was treated with copper anode current densities of 13.73 A/m^2 and 21.9 A/m^2 and ink concentration of 0.088 mg/mL was treated with aluminum at the same anode current densities. Higher current densities and acidic conditions had higher decontamination efficiency. The wash filtrate was treated with aluminum anode at current densities of 6.87A/m^2 and 13.73A/m^2. Unlike the model flexographic ink dispersion, pH changes induced coagulation in the untreated wash filtrate. The destabilization of inks dispersions was aided by metal ions and protonation at acidic pH. Under acidic environment, the carbon black ink particles are more hydrophobic and bubbles generated by the electrolysis of water easily collect these inks. A comparison of anode electrodes, show that the copper electrode gave higher decontamination efficiency than aluminum electrode.

Investigating the Anatomical Features of Ethanol Organosolv Pretreated *Buddleja davidii*.
Author: Bassem Hallac
Email: bhallac3@gatech.edu
Advisor: Art Ragauskas
Abstract: In the bioconversion process of biomass to bioethanol, pretreatment is considered to be the crucial step because it governs the susceptibility of the biomass to the downstream hydrolysis and fermentation. The exact effects of pretreatment on biomass are not completely understood. This study provides information on the anatomical characteristics of *Buddleja davidii* substrate after ethanol organosolv pretreatment that can be responsible for efficient cellulose hydrolysis of cellulose by cellulases. Results showed that the ethanol organosolv pretreatment of *B. davidii* selectively removes lignin in the middle lamella (ML), causes cell deformation, and

cracks or breaks the cell wall, while retaining the crystallinity of cellulose. The removal of lignin from the ML regions was the most pronounced microscopic observation and believed to be the major factor for efficient enzymatic hydrolysis. The enzymes were able to penetrate easily through the outer part of the cells where the ML was absent.

Fiber Modification via Starch Grafting for Improved Paper Properties

Author: Delong Song
Degree program: PhD in Paper Science and Engineering
Email: dsong3@gatech.edu
Expected graduation date: May 2011 Faculty advisor: Dr. Yulin Deng

Abstract: A facile method to graft biodegradable starch onto fiber surfaces through the hydrogen bond formation among cellulose, starch and ammonium zirconium (IV) carbonate (AZC) was developed. The effects of grafting conditions, including pH, temperature, fiber consistency, crosslinker, starch dosage and mechanical agitation on the grafting yield were systematically investigated. Optical and electron microscopes clearly revealed that, after grafting, the fiber surface was covered by a hydrogel of starch. It is believed that the grafted starch functions similarly as wood fibrils generated by refining. We found that, compared with the paper sheets made of fibers with an industry refining level (420 ml CSF), the paper sheets made of fibers with a much lower refining degree but with grafted starch showed higher paper strengths, including tensile strength, stiffness and z direction tensile (ZDT); meanwhile, a higher drainage rate was also achieved.

Development of New Gasification Processes for Biomass Residues: Gasification Kinetics at Pressurized Conditions

Authors: Gautami Newalkar and Abiola Shitta
Email: gnewalkar3@gatech.edu and ashitta3@gatech.edu
Advisers: Dr. Pradeep Agrawal and Dr. Carsten Sievers
Degree Program: PhD in Chemical and Biomolecular Engineering/PSE students
Expected Graduation: December 2014

Abstract: A major advantage of biomass gasification is that waste and residue from forest and paper industry can be converted to syngas. Biomass gasification involves pyrolysis and char gasification steps in series. Key parameters include ash content, temperature, pressure, and heating rate. The present study aims to develop kinetic models for high pressure gasification of loblolly pine, switchgrass, and cornstover using:(i) pressurized entrained flow reactor (PEFR) with high heating rates (≥ 10^3 ^oC/sec) and short residence times, and (ii) pressurized thermo-gravimetric analyzer (PTGA) with lower heating rates, but larger residence times (5-100 min). The char yield and its gasification activity are affected by the pyrolysis pressure, temperature and heating rate. CO_2 gasification studies of char show the chars generated in PEFR to be more active than those from PTGA. The char gasification data are coupled with transport effects. Attempts to build mathematical models are presented.

Fate and Degradation of Sterols in Pulp Mill Wastewater

Author: Hamilton Giles
Email: hgiles3@gatech.edu
Advisors: Spyros Pavlostathis and Sujit Banerjee
Degree Program: Environmental Engineering
Expected Graduation Date: May 2013

Abstract: Pulp mill wastewaters have been found to cause hormone (endocrine system) related changes in fish present in receiving waters. Sterols are suspected of being the major contributors to the endocrine disrupting potential of the wastewater. Aerated stabilization basins are widely used in the pulp and paper industry for the treatment of wastewater. The tapered aeration that is used in these systems lead to the presence of several redox environments within the same treatment system. (Environments such as aerobic, methanogenic and sulfate reducing). The goal of this research is to determine the fate and biodegradation potential of sterols within the different redox environments present in aerated stabilization basins. The effect of different treatment conditions on the overall endocrine disrupting potential of the wastewater and how that correlates to sterol fate and degradation will also be examined.

Design of Robust and Smart Antimicrobial Microcapsules from Double Pickering Emulsions for Application in Paper and Packaging

Author: Hongzhi Wang
Email: hwang97@gatech.edu
Advisor: Dr Sven. Behren
Expected graduation year: 2013

Abstract: In a two-pronged approach, we investigate the fundamentals of emulsification with colloidal particles and apply the obtained insights to the design of emulsion-templated microcapsules with customizable properties for antimicrobial modification of paper and packaging materials. The fundamental part of the project focuses on understanding the prerequisites for decorating and stabilizing emulsion droplets with charged colloidal particles. Such particle-covered droplets are used, in the applied part of the project, as precursors for a new type of microcapsules suitable for efficient encapsulation of antimicrobial substances. The investigated capsules are designed to withstand the pressure, shear and thermal stresses encountered in papermaking and printing processes, while offering the benefit of sustained release or triggered release of their antimicrobial cargo in response to external stimuli such as pH, temperature, or, possibly, microbial attack. Specifically, the suitability of such microcapsules for the post-production functionalization of packaging surfaces by flexographic printing shall be explored.

Stereochemical Dependence on Bioactivity of an Inhibitor of Loblolly Pine Somatic Embryogenesis and Work in Progress Identification of a Substance Stimulatory to Loblolly Pine Somatic Embryo Germination

Author: Jacob Lucrezi
Email: jlucrezi3@gatech.edu
Advisor: Sheldon W. May
Degree program: PhD in biochemistry from the School of Chemistry and Biochemistry
Expected graduation date: Summer 2012

Abstract: Somatic embryogenesis (SE), a vegetative propagation program reproducing whole plants from callus and suspension cultures, has become the most promising for propagating superior genotypes. The unattached haploid female gametophyte (FG) surrounding the diploid zygotic embryo is not present in embryogenic tissue culture. Previously we had identified, evidence that *myo*-inositol-1,2,3,4,5,6-hexa*kis*phosphate ($InsP_6$) is produced in FG of Loblolly Pine from late stages (9.9-9.12) and that it can suppress early stage somatic embryo growth and multiplication. Here we present, evidence that *muco*-inositol-1,2,3,4,5,6-hexa*kis*phosphate (*m*-$InsP_6$) does not affect early stage somatic embryo growth and multiplication. Previously we had identified, evidence that FG of Loblolly Pine from middle stages (8-9.2) can generate substance(s) that are able to advance somatic embryo maturation resulting in increased germination. We show in-progress results in the attempt to isolate and identify the substance(s) that account for this activity via the use of HPLC and bioassays.

Tar Reforming of Biomass Derived Syngas

Author: Jessica Ewbank
Email: jle3@gatech.edu
Advisor: Carsten Sievers
Degree Program: Department of Chemical & Biomolecular
Expected Graduation: May 2015

Abstract: Biorenewable resources present a promising opportunity for the production of sustainable and carbon-neutral fuel. One very viable renewable energy resource is lignocelluslosic biomass. This renewable resource can be gasified, reformed, and ultimately transformed into biofuels via Fischer Tropsch Synthesis. One of the major issues still facing this promising technology is reforming of the biomass derived syngas. Biomass derived syngas contains a high amount of tar and these tars can condense in process lines causing fouling and clogging of equipment downstream of the gasifier. Additionally, biomass may also contain large amounts of sulfur, which poisons catalysts used in the reforming as well as in Fischer Tropschs process. Our work focuses on reforming of tars in biomass derived syngas problem. We aim to create a catalyst with excellent selectivity for tar reforming and superior sulfur resistance.

White Coatings from Renewable Resources for Sustainable Paper and Paperboard Products

Author: Jie Wu
Email: jwu71@gatech.edu
Advisor: Carson Meredith
Degree Program: PhD Student, School of Chemical and Biomolecular Engineering
Expected graduation date: Summer of 2013

Abstract: Paper and paperboard require significant whiteness and brightness. Traditional approaches to attain that goal have included lignin extraction, addition of mineral fillers and bleaching treatments that involve energy-intensive processes that produce additional waste streams and add additional mineral mass in the final product. A recent discovery indicates that a three-dimensional random network structure makes the white beetle have high whiteness and brightness. The goal of our study is to develop assembly methods for reproducing this white beetle scale structure synthetically and extend this approach to coat paper and paperboard products. The preliminary results show that it is possible to fabricate network structure at white

beetle scale.

Effect of Chlorides on Selective Corrosion and Stress Corrosion Cracking of Duplex Stainless Steels in Simulated White Liquor

Author: Kevin R. Chasse
Email: Kevin.chasse@gatech.edu
Adviser: Dr. Preet M. Singh
Degree Program: PhD in Materials Science/PSE minor

Abstract: "The current work evaluated the role of chlorides on stress corrosion cracking (SCC) and selective corrosion of standard grade UNS S32205 and lean grade UNS S32101 duplex stainless steels (DSSs) in simulated white liquor at 170 ^{0}C. Test solutions contained 100 – 150 g/L NaOH, 50 – 75 g/L Na_2S, and 0-100 g/L NaCl. Susceptibility to SCC and selective corrosion were evaluated through weight loss testing and constant extension rate testing. Samples were characterized with scanning electron microscopy (SEM), optical microscopy, X-ray photoelectron spectroscopy (XPS), and energy dispersive spectroscopy (EDS). A significant change in fracture morphology is observed when chlorides are added to alkaline sulfide solution. Chlorides enhance selective dissolution of the austenite phase for concentrations of NaCl (0.5–10 g/L). Sulfides and polysulfides adhere to the surface of DSSs in hot alkaline sulfide solution, which leads to defective passivation, particularly in the presence of NaCl."

Accelerated Hydrolysis of Starch for Production of Biofuels

Authors: Kendra Maxwell and Sandeep Mora
Email: kmaxwell@gatech.edu and sxm3645@gatech.edu
Advisor: Dr. Sujit Banerjee

Abstract: Improved efficiency in the hydrolysis of starch to glucose is key to reducing energy use during the conversion of starch to bio-fuels and other bio-materials. It has been found that the addition of a positively charged polyelectrolyte increases the conversion rate of starch to glucose. A combination of analytical methods was used to study the interaction between polyelectrolyte, starch, and enzyme components in order to determine their effect on hydrolysis rate. In addition, viscoelastic effects caused by starch gelatinization are examined. Results indicate interactions caused by electrostatic forces drive the increase in hydrolysis rate.

Effects of Ethanol Fuel Chemistry on the Stress Corrosion Cracking and Passivation of Pipeline Steel

Author: Lindsey Goodman
Email: lindsey.goodman@gatech.edu
Advisor: Dr. Preet Singh

Abstract: Growing interest in the use of alternative fuels has led to an increase in production of fuel grade ethanol (FGE), necessitating an efficient method of transportation for this biofuel. Occurrences of stress corrosion cracking (SCC) of pipeline steels in FGE have spurred studies toward understanding the phenomenon of this environmentally assisted corrosion. Prior work in simulated fuel grade ethanol (SFGE) has shown that water, chloride ions, dissolved oxygen, and acidity are all major factors in the promotion of SCC of pipeline steel. In this research, passive film characteristics and passivation kinetics of X65 pipeline steel in FGE environments are explored. Results of scratch tests performed to compare passivation kinetics of X65 steel in FGE environments containing chloride and water are described. Based on experimental results, limiting parameters for SCC occurrence in FGE environments are discussed.

Fabrication of a Cellulosic Nanocomposite Scaffold with Improved Supermolecular Structure as a Potential Cardiovascular Tissue-Engineered Graft

Author: Parisa Pooyan
Email: parisa.pooyan@gatech.edu
Advisor: Cyrus Aidun and Hamid Garmestani

Abstract: Cellulose nanowhiskers (CNWs) with its renewable and environmentally benign nature, and its abundance and excellent biocompatibility could potentially open a new avenue in

cardiovascular tissue engineering for small caliber grafts. Inspired by this bioapplication, we have designed a fully bio-based nanocomposite of aligned CNWs embedded in a matrix of cellulose acetate possessing a controlled biodegradability, 3D porosity, and non-acidic byproducts as opposed to degradable PLA/PGA. To ensure uniform distribution, CNW were delicately extracted from a multi-stage process and dissolved in a solvent of choice prior to mixing with the matrix to inhibit whiskers flocculation. Comparable to Carbon Nanotubes and Kevlar, CNWs imparts significant strength and directional rigidity to the composite even at 0.2 wt% yet intensifies to about fourfold within a controlled magnetic field of 0.3T. We believe our novel aligned nanocomposite could have ground-breaking features withstanding the physiological pressure and mimicking the topographical texture of the native extracellular graft.

Engineering Cellulolytic Escherichia coli towards Biofuel Production

Authors: Ramanan Sekar, Dr. Hyun-Dong Shin, Dr. Rachel Chen
Email: rsekar6@gatech.edu
Advisor: Dr. Rachel Chen
Degree Program: Master of Science in Chemical and Biomolecular Engineering
Expected date of Graduation: Summer 2011

Abstract: The current energy crisis is exponentially growing and widening the chasm between demand and supply. Biofuels such as ethanol not only provide greener alternatives to fossil fuels but have been shown to reduce emissions from vehicles, improving air etc. Biofuel production from sources such as cellulose is believed to be more sustainable due to its low cost, vast availability in nature and sources such as industrial plant waste can be put to good use. However, due to the absence of a low-cost technology to overcome its recalcitrance, a concept called Consolidated Bioprocessing (CBP) has been put forward which proposes to integrate the production of saccharolytic enzymes, hydrolysis of the carbohydrate components to sugar molecules, and the fermentation of hexose and pentose sugars to biofuels into a single process. The present study involves development of cellulolytic *E. coli* strains towards cellodextrin assimilation by employing an energy-saving strategy in cellulose metabolism through the phosphorolytic cleavage of cellodextrin mixture produced as cellulosic degradation products.

Hydrodeoxygenation of Pyrolysis Oils

Author: Sarah McNew
Email: gth698k@gatech.edu
Advisor: Carsten Sievers

Abstract: Pyrolysis oils are complex mixtures that can be obtained from any biomass source. Oxygen is a primary component of these oils and contributes to the limited storage stability, corrosiveness, and high viscosity. Based on these facts, pyrolysis oils must be upgraded to improve storage and fuel properties for real world use. Hydrodeoxygenation replaces oxygen containing groups by hydrogen with water as the only side-product. In principle hydrodeoxygenation can be performed with hydrodesulfurization catalysts from petroleum refineries. These catalysts contain defect sites that bind and remove sulfur or oxygen from organic molecules. However, when the catalysts are used for hydrodeoxygenation toxic hydrogen sulfide must be supplied to keep them in their active form. We are designing a new, sulfur-free catalyst for use in hydrodeoxygenation with comparable properties to the catalysts used in hydrodesulfurization.

Understanding Aspect Ratio Effects on Polymer Crystallization and Mechanical Properties in Cellulose/ Polyhydroxybutyrate Nanocomposites

Author: Stephanie Lin
Email: Stephanie.lin@gatech.edu
Advisor: Meisha Shofner

Abstract: In this research, cellulose nanocomposites will be produced using a naturally-derived polymer, polyhydroxybutyrate (PHB) to test the hypothesis that anisotropic nanofillers can be used to increase mechanical modulus and toughness concomitantly through manipulation of self-seeding crystallization in PHB. If successful, this research will lead to the development of new

materials with reduced environmental impact and unique combinations of properties that are not available in other materials. Additionally, the specific materials proposed will provide opportunities to increase the application range of PHB polymers and more fully understand the impact of nanoparticles on crystallization and mechanical properties in highly crystalline systems. This fundamental understanding will also provide insight into structure-property relationships in other types of polymer nanocomposites and suggest guidelines for composite design.

Catalytic Study on Bio-mass Hydrogenation and Conversion into Biofuel

Author: Wei Mu
Email: muw0@gatech.edu
Faculty advisor: Professor Yulin Deng
Degree Program: Ph.D in Chemical Engineering Department
Expect graduation date: August 2013

Abstract: Catalysts have played an important role since it was invented. It greatly reduced the energy consumption, efficiency and selectivity in the manufacturing process. My research is focusing on the catalyst design to convert the biomass into biofuel. In my experiment, I mainly studied hydrogenation catalysts, like Ruthenium and Nickel. Both of them could greatly reduce the unsaturated bond in the biomass and producing the aliphatic compound. It could also break the large pieces of molecular into very small one which could be used as the transportation fuel.

Water-Driven Shape Memory Aerogel from Crosslinked Native Cellulose Nanofibers

Author: Yaan Zhang
Email: yzhang335@gatech.edu
Advisor: Dr. Yulin Deng

Abstract: Aerogels are ultra-lightweight materials with a highly porous network structure. Cellulose aerogels have additional advantages of biocompatibility and biodegradability but they feature properties similar to inorganic counterparts. In our experiment, we investigated a robust aerogel from chemically crosslinked native cellulose nanofibers prepared by freeze-drying, which show extraordinary superabsorbency and interesting shape memory properties driven by water controlled hydrogen bonding between cellulose nanofibers. The structure is hierarchical porous with pore size ranging from nano- to macro- scale. The water-driven shape recovery can be regarded as a polymer swelling process during which small molecules permeate into cellulose matrix. The results of this work contribute such bio-based, bio-degradable, and environment-friendly nanomaterials to a broader application field, such as water retaining materials in agriculture, templates for further modification, tissue engineering, smart drug delivery system, etc.

Effect of Steam Explosion on Degradability and Accessibility of Loblolly Pine for Biofuel Applications

Authors: Yuzhi Kang, Prabuddha Bansal, Matthew Realff, Andreas Bommarius
Email: ykang41@gatech.edu
Advisors: Matthew Realff, Andreas Bommarius
Degree: PhD Student, School of Chemical and Biomolecular Engineering,
Expected Graduation: May, 2013

Abstract: Among the various biomass pretreatment methods, steam explosion is one of the most widely used due to its cost-effective disruption of the plant structure and hence enhanced enzymatic accessibility. Three different substrates, Avicel, phosphoric acid swollen cellulose (PASC), and SO_2 steam-exploded loblolly pine (SELP), were subjected to enzymatic hydrolysis and subsequent adsorption study. Despite the complexity of both substrate and enzyme mixtures, the SELP adsorption isotherm can be fitted to Langmuir equation ($R^2 > 0.97$). The saturation point was reached at ~6.24 mg/ml total enzyme loading. Adsorption data were also correlated with initial rates and once again showed the dependence of initial rate on initial adsorption amount.