

Master of Engineering Projects - 2009

Purpose

The purpose of the Masters of Engineering Project is to apply knowledge acquired in the M. Eng. Program to a specific application of industrial, biological, or environmental importance. The project integrates chemical engineering science, design, and, in some cases, economics, to accomplish specific goals, such as development of innovative technology, refinement of new analytical tools, or improvement of material properties and processing characteristics.

New M. Eng. students may select a project in their chosen area of concentration from a list of possible projects developed by the faculty. Alternatively, students may suggest a project of their own design.

Students will tentatively select a project by **November 1**. Project selection will be finalized by **December 1**. Multiple students may work on a project as a team with the consent of the Project Sponsor.

Each student must present a project proposal to their Project Sponsor and receive approval to proceed. Also, each student or group of students must meet with their Project Sponsor at the start of the project and present a project execution plan following the format given below (if the Project Sponsor requires this).

As a minimum, students will meet with their Project Sponsor at each of the milestones described in the project execution plan. At these meetings the student(s) and the project sponsor should discuss progress to date, work to be accomplished before the next milestone, estimate of effort to complete the work, potential areas of concern which could affect completion of the plan and any outstanding issues from previous meetings.

Deliverables

The deliverables for the M. Eng. Project are as follows:

- Project Proposal
- Project Execution Plan
- Interim Report
- Final Report
- Oral Presentation

Project Proposal

The project proposal should include the following:

- Background
- Statement of the specific problem including why the project constitutes an improvement over current technology or practice.
- Economic drivers and the potential economic advantages, if applicable.
- Methods to solve the problem.
- Factors, milestones, or outcomes that define success.

Project Execution Plan

The project execution plan should include the following:

- Description of work plan.
- Milestone schedule
- Resources required
- A draft of the final report's Table of Contents

Testing a New Theory of Rubber Elasticity (Claude Cohen)

Rubber is made of flexible long-chain molecules tied together covalently by small molecules (crosslinks) forming a 3-dimensional network. At equilibrium, a flexible polymer chain takes on many random conformations corresponding to a state of higher entropy. When a rubber is stretched, its constituent polymer molecules are extended and possess less entropy. If the force exerted on the rubber is removed, the stretched rubber snaps back to its original state to maximize its entropy. Although classical theory of rubber elasticity can describe the behavior at small deformations, it fails at large deformation. A recently developed model by physicists (Physical Review Letters 98, 075502, 2007) included thermal fluctuations (random molecular motions) of the chains and crosslinks that were previously neglected. This theory appears to account better for the observed experimental results at higher deformation.

This project consists of analyzing experimental data obtained on a series of carefully synthesized polydimethylsiloxane elastomers in our laboratory in terms of this new theory. In addition to the analysis of available data, mechanical testing (obtaining stress-strain curves) of existing samples and possibly synthesizing some more samples may be required to complete the project.

Growth of supracrystals (Tobias Hanrath)

In broad terms, this project explores the self-assembly of nanomaterials into highly ordered structures. As in the familiar atomic crystals, collective interactions among nanocrystals assembled in an analogous 'artificial solid' are strongly influenced by nanocrystal energy levels, by coupling between adjacent sites, and by the symmetry and spacing of the lattice. Similarly, the project draws on many important lessons from the assembly of micrometer-sized colloids into supracrystals. At the intermediate length scale, the grand challenge facing nanotechnology is to assemble nanomaterials building blocks into robust and scaleable structures in which they can interact in purposeful ways. Specifically, the project involves combining an automated dip-coating system with horizontal linear-stage convective assembly to explore whether atomic-scale principles such as epitaxial growth, lattice mismatch and interface strain can be applied to the growth of nanocrystal supracrystals.

Nano-composite silicone lubricants (Lynden Archer and Claude Cohen)

Polymer network lubricants made with polydimethylsiloxane (PDMS) were shown by our group to significantly reduce the coefficient of friction (COF) of solid surfaces. The COFs that we have determined for these PDMS lubricants are among the lowest ever recorded for dry systems. In order to further improve on the properties of these lubricants, we are planning to introduce surface-modified silica nanoparticles into the precursor polymer chains before crosslinking occurs. We anticipate that the nanoparticle fillers would decrease interfacial contact area, thus helping to reduce the contribution of adhesion to the overall friction force. Furthermore, silica particles are known to improve the tear properties of elastomeric materials and are used extensively for this purpose in industry.

This MEng project consists of synthesizing nanoparticle organic hybrid materials (NOHMs) to be used as fillers for PDMS lubricants. The core silica particle will be modified with polyethylene glycol oligomers to which longer PDMS chains will be attached. The modified nanoparticles would be compatible with the PDMS chains that form the lubricant matrix. The MEng student will be instructed in the synthesis of NOHMs with various surface density and chain lengths and their incorporation in the lubricant systems. Characterizing the micro- and macroscopic frictional properties of various composite lubricant systems will be part of the project.

A student with interest in polymers and new materials would be ideal for this project. He/She will gain a greater understanding of the chemical and physical properties of both nanoparticles and polymer systems.

Carbon Capture using New Task-specific Ionic Liquids (2 positions available) (Lynden Archer)

Ionic Liquids (ILs) are organic salts with melting points below 100°C. These salts generally consist of a bulky organic cation and an inorganic anion. The large cation size causes delocalization and screening of its charge, resulting in a low lattice energy and unusually low melting point or glass transition temperature. Ionic liquids exhibit many interesting properties, which make them suitable for applications as solvents in chemical synthesis, catalysis, electrochemical applications and gas separations. Knowledge of the solubilities and diffusivities of gases in ILs is of interest for a number of applications. Gas solubility is vital for carrying out reactions such as hydrogenations, hydroformylations, and oxidations involving permanent or condensed gases in IL solutions. The design of gas separation processes involving ILs requires gas diffusivity data. Among the different gases, carbon dioxide is the most widely studied for application of ILs in separating carbon dioxide from flue gas streams.

The objective of this project is to characterize absorption and transport of CO₂ in two families of ionic liquids. One family is composed of bulky organic cations with inorganic counterions, the other utilizes charged inorganic nanostructures as the cation and organic oligomers (short polymers) as the counterion. Using time-dependent measurements of pressure in a closed, thermostated chamber containing CO₂ in contact with the IL, we will determine the solubility, H ,

and diffusivity, D_{AB} , of CO_2 in a variety of ILs. Specifically, by fitting the measured time-dependent pressure profile to a model for one dimensional diffusion of a gas into a liquid film, we will compute the Henry's law constant H and D_{AB} for ILs with a variety of appended chemical functionalities (e.g. aliphatic amines and esters). These measurements will be complemented with rheological characterization of the ILs to determine their temperature-dependent viscosity $\eta(T)$ and flow activation energies, E_a . By comparing the observed dependence physical properties (H , D_{AB} , η and E_a) on chemical functionality, we propose to develop new families of ionic liquids that can be used for cost-effective capture of CO_2 emissions from fossil-fuel burning power plants.

Potable Water Recovery from Humid Air (AI Center)

There are many parts of the world where potable water is scarce and the air temperature and the humidity are both high. In many cases these areas do not have well developed infrastructures and thus potable water produced by multi-effect evaporation or reverse osmosis desalination must be brought over long distances from the production site to the consumer. This is frequently not a viable option.

It has been suggested that small potable water supply systems could be put in place that would recover water from the atmosphere by condensation from the ambient air. It has further been suggested that the chilling system would use ammonia absorption or some such similar system that required little or no mechanical energy and might take advantage of solar thermal power to supply some of the energy to run the chilling system.

Your task is to develop a standalone system based on recovery of water from humid air that would produce potable water for a village of 1000 with minimal external energy supply.

Refinery Modeling (AI Center)

A comprehensive refinery model has been under development for several years. This model is still rudimentary and does not reflect current US product quality requirements. It is also not all that user friendly.

The task will be to upgrade the model to make it representative of current product market conditions, to add ethanol blending to gasoline and to make it transparently user friendly.

A copy of the model and the instructions for use can be found on Blackboard.

An Oxygen-Based Approach the Claus Process (AI Center)

Hydrogen sulfide is a byproduct of natural gas processing and petroleum refining. The hydrogen sulfide is converted to liquid sulfur via the Claus Process. In the Claus Process, the hydrogen sulfide is burned in air to produce a mix of sulfur dioxide and hydrogen sulfide.

The initial reaction occurs in a combustion chamber and about 60% of the hydrogen sulfide is converted. The reaction mass is cooled and liquid sulfur precipitates from the reaction mass and is removed. The remaining reaction mass is reheated and passed over a catalyst bed where approximately 60% of the remaining hydrogen sulfide is converted to sulfur. The reaction mass is cooled, liquid sulfur condenses and is removed. This catalytic step is repeated a second time and the reaction mass now contains about 3% of the sulfur fed to the process.

At this point the gas stream is so dilute in sulfur that the partial pressure of the sulfur is equivalent to the vapor pressure of solid sulfur. This precludes any further removal by condensation. At this point the reaction mass is fed to another process called the SCOT Process which removes the remaining 2+% sulfur. The SCOT Process is equal in capital cost to the Claus Process.

A possible alternative to the SCOT Process would be to feed the Claus Process with an oxygen rich stream obtained by passing air across a membrane that would separate oxygen and nitrogen. There would, therefore, be far less total mols of gas and the partial pressure of sulfur would be higher.

Full details of the Claus Process may be found in Chapter 22 of the GPSA Handbook.

The objective of the project is a reaction engineering study to determine the viability of this concept. The study should recommend the appropriate level of oxygen enrichment, the design basics of the new reaction scheme and some idea of how the cost might vary from a conventional Claus Process.

Salt Water Algae as a Source of Bio Fuels (AI Center)

Cellera Corporation is investigating the large-scale, on-shore cultivation of algal colonies. Some algal types are fairly high in lipids. The process that seems most promising at this point is high temperature hydrolysis of the algal mass, producing free fatty acids, glycerol and denatured cell mass.

The free fatty acids can be converted to the methyl ester and be used as a replacement for petroleum derived diesel. This is attractive, firstly, because all petroleum diesel is presently either imported or produced from imported crude, and, secondly, because the methyl ester fuel is easily biodegradable relative to petroleum diesel.

There is a large residue of cellular material, which will probably be best converted to incremental energy by biodigestion.

The objective of this project is to determine the most cost effective method to win free fatty acids and glycerol from the algae. The project should also evaluate the best value recovery scheme for the residual cellular material.

Compressed Air as a Means of Energy Storage (AI Center)

One of the problems arising from the use of either solar or wind generated electrical energy is the variability of supply. Another problem is that the energy is usually produced in an area of low energy demand and, thus, the electricity must be transmitted over long distances to the consumer.

A possible solution to these problems is to compress air at the point of power generation and to replace the compression section of the typical power generating gas turbine with compressed air delivered by pipeline. Compressing the air to a higher pressure than needed by the gas turbine will allow volume to be stored in the pipeline as “line pack” and to be readily available to the gas turbine as electrical demand swings.

The project should look at the facilities required to make this a viable idea and to produce an estimate of capital and operating costs for the facilities that translate back into a cost per kilowatt for the supplied power.

Recovery of Hydrocarbons in a Depleted Producing Field by in-situ Gasification (AI Center)

Using oxygen to convert coal seams into synthesis gas by partial combustion has been a demonstrated but not commercialized technology for many years. Since depleted oil and gas fields may contain more than half the total hydrocarbon originally in place in the formation, it may be possible to recover a significant amount of the energy potential of the hydrocarbons in place by methods and technology similar to Underground Coal Gasification. This project will require a fair amount of geological knowledge and so might best be done with a partner from Earth and Atmospheric Sciences.

**Modeling and Design of the Thermophysical Properties of
Novel Nanoparticle-Organic Hybrid Liquids
(Fernando Escobedo)**

This project entails the use of advanced modeling software to predict and correlate the thermodynamic and rheological properties of novel solvent-less fluids containing inorganic nanoparticles whose surfaces have been functionalized with suitable organic oligomers. Such materials are the object of intense experimental studies by several groups at Cornell and elsewhere for potential applications involving, for example, the capture of CO₂ and organic gases and for water purification. This project is part of a joint effort to provide a more fundamental basis to the rational design of these new class of materials.

**Unveiling the Folding-Unfolding Mechanism of Proteins
(Fernando Escobedo)**

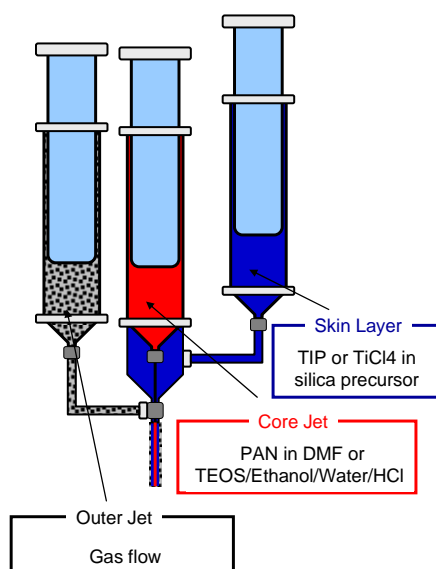
Unlike most modeling studies of protein mutants that have focused on predicting the structure of the folded state, this study aims to understand the folding process by identifying (and potentially learning to design) the “transition states” or intermediate gateways that explain the different fates that the product can take. Studies of this nature can help rationalize and overcome the low yields of active protein often observed in engineered protein production operations. This project entails the use of new molecular simulation methods to describe the kinetic mechanism by which proteins, such as nanobodies, fold and unfold. Nanobodies are a type of minimalistic antibody (derived from Camelids) that surpass conventional antibodies for some biotechnological applications. This is because nanobodies are known to be very robust folders (resisting different denaturing conditions such as heating) and very versatile binders (binding to hidden sites). This study could thus provide further insights for the use and design of new nanobody mutants.

**Design of Gas Assisted Electrospinning for Multi-axial Jets
(Yong L. Joo)**

Electrostatic fiber spinning or ‘electrospinning’ is a novel process for forming fibers with submicron scale diameters through the action of electrostatic forces. When the electrical force at the interface of a polymer liquid overcomes the surface tension, a charged jet is ejected. The jet initially extends in a straight line then undergoes a vigorous whipping motion caused by the electrohydrodynamic instability. Finally, the jet solidifies into nanofibers. Nanoscale fibers produced by electrospinning are finding uses in various applications including filtration, protective clothing and biomedical applications. In our group, we have been developing multiaxial electrospinning for multi-layered nanofibers. One of the main drawbacks of multi-axial electrospinning is its low productivity. To increase the productivity of multi-layered nanofibers, gas assisted electrospinning will be adapted to our facilities. It has been demonstrated that the nanofiber production rate can be increased by ten times while keeping the fiber diameter the same. At a fixed flow rate, the fiber diameter can be smaller with this approach. Gas flow can easily be incorporated into coaxial scheme where additional skin layer (and thus it becomes

triaxial jets) will be a gas flow to produce coaxial nanofibers at a much faster rate. A triaxial electrospinning has been utilized in the confined assembly of block copolymers sandwiched by silica layers in our group, and we will modify our existing triaxial setup to incorporate gas flow into coaxial jets for higher production rate of coaxial nanofibers (see the figure below).

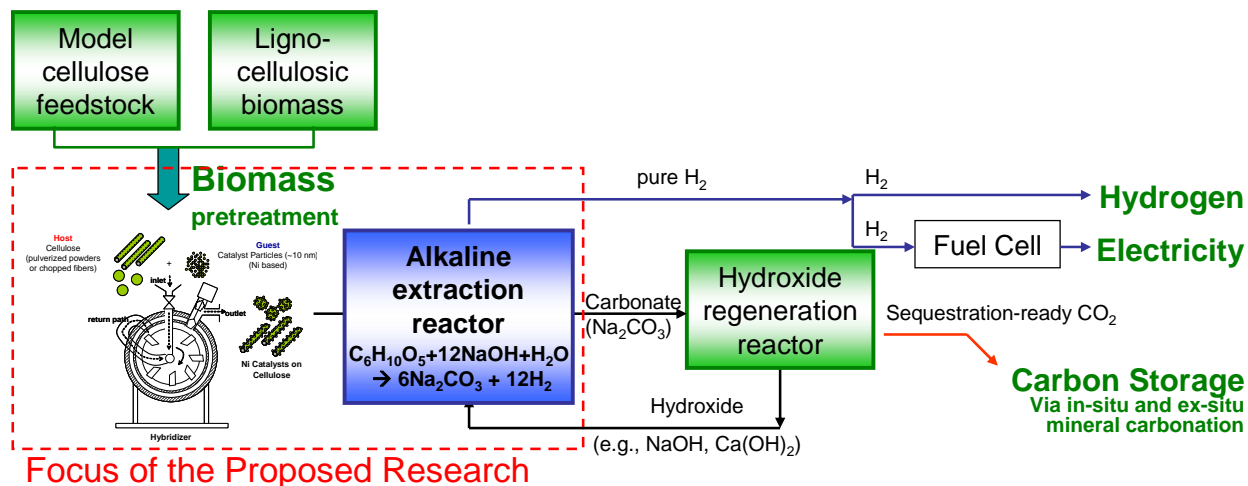
**Biomass Refining System via Alkaline Hydrothermal Treatment Technology:
Pretreatment and Catalyst Development
(Yong L. Joo)**



We have been developing a small rural or farm-scale biorefining system that can convert engineered algae and/or farm wastes into hydrogen (H_2) and electricity. In particular, we will focus on the development of effective procedures for biomass pretreatment and catalysts for alkaline hydrothermal treatment. Compared to conventional gasification and pyrolysis, the proposed alkaline hydrothermal treatment is a less-studied method of biomass conversion but with great potential. Unlike in biogasification, which results in a mixture of H_2 and CO , which can damage the electrocatalysts at the anode of a polymer electrolyte cell, the H_2 generated in an alkaline hydrothermal reactor will have a purity that would be suitable for direct application in a fuel cell. For optimization of feedstock utilization and processing, biomass pretreatment and catalyst development are essential. To this aim, i) the effect of hydrolysis pretreatment of well characterized cellulose on alkaline hydrothermal reaction will be studied first. To maximize the catalyst loading while minimize the overall catalyst requirements, ii) the synthesis of Ni catalysts in cellulose biomass via treatment with Ni precursors followed by chemical reduction, and and iii) utilization of inorganic (silica, alumina, titania) nanofibers containing Ni catalysts on their surface at the catalyst system will be investigated. The proposed process will eventually be integrated with carbon capture and storage (CCS) technology, which can further improve the environmental sustainability of the biomass conversion. Alternatively, this scheme can be integrated to the existing Fischer-Tropsch (F-T) process to produce more diversified liquid

products. Our ultimate objective is to create the scientific and engineering foundation for a transformative solution for mass-producible, sustainable energy production from biomass.

Green Nanofilters based on Proteins from Natural Resources (Yong L. Joo)



With the spread of the H1N1 (swine flu) virus over the past few months, there are legitimate concerns about the occurrence of a worldwide influenza pandemic. In the event of such a pandemic, limitations on the supply and distribution of vaccines and antiviral drugs imply that disrupting the transmission of the influenza virus needs to be a viable alternative strategy. Developing strategies requires one to understand the transmission modes of the airborne virus and interrupt it. By combining high surface area of biodegradable fibers and biologically active components in soy and whey proteins, we propose to develop novel nanofilters based on green materials which can capture and destroy airborne viruses including influenza virus. To this end, we will electrospin the mixture of protein isolate and solution of biodegradable polymers such as cellulose, polyvinyl alcohol and polylactic acid on the conventional filter media to increase filtration efficiency of submicron scale dust particles. The biologically active component in protein isolate such as sialic acid can act as an effective receptor for influenza virus capture. The quantifying virus capturing efficiency will be carried out in two folds. First, a viral infectivity assay such as a plaque assay will be employed to a model system based on reoviruses in collaboration with Prof. John Parker at the Baker Institute of Animal Health. The basis of the plaque assay is to measure the ability of a single infectious virus to form a “plaque” on a confluent monolayer culture of cells. Secondly, we will use quantitative RT-PCR to quantify the amount of viral genome (double-stranded RNA). The sensitivity of virus detection will be aided by Professor Antje Baeumner in Biological & Environmental Engineering at Cornell. After satisfactory filtration efficiency for model viruses is achieved, we intend to test out filter media for filtration efficiencies of influenza virus in collaboration with Dr. Laura Kramer, Director, Arbovirus Laboratories at Wadsworth Center in New York State Department of Health.

**Energy Management at Wireless Cell Site Installations –
Analysis and Simulation of Geothermal Heat Pump Utilization
(J. Tester)**

Rising energy costs and the desire to mitigate the harmful impacts of energy use on the environment have caused us to look hard at the energy efficiency of our cellular network. Energy consumption at cell sites contributes significantly to our total energy consumption as an enterprise and we are currently working on a number of strategies to improve the energy efficiency of our cell sites. One opportunity that has been identified is the use of free cooling strategies such as the use of air-side economizers. Although this method of free cooling has its benefits, it doesn't work in all climates and the solution's reliability can be negatively impacted by environmental conditions. Project will explore viable options for vertical well closed-loop ground source geothermal heat pump systems to be used for "cooling ONLY" applications at cell sites with 5-ton or less peak cooling demands.

**Life cycle analysis of high lipid algal biofuel processes from
feedstock production to biofuel utilization
(J. Tester, Brad Anton, Beth Ahner, Larry Walker)**

Quantitative analysis of mass and energy flows and their impact on net process efficiency in the context of technical and economic feasibility. Aspen Plus or similar process simulation software will be used to model processes. Scale up for deployment to meet national level goals, water and land use and other environmental issues, assessment of impacts on carbon and nutrient cycles, and process robustness will need to be evaluated. A range of options for conversion of biomass feedstocks to fuels and other products such as animal feed should be considered. These would include conventional biodiesel processes and biochemical transformations as well as hydrothermal liquefaction.

**Evaluation of Geothermal Potential in the Eastern United States
(J. Tester, Larry Brown, Terry Jordan)**

Analysis of geothermal resource potential based on geologic information including heat flow, bottom hole temperatures, in situ stresses, rock types and properties as a function of depth in the Northeast region for New York, Pennsylvania and the New England States to evaluate end use potential for direct use, electric power, co- generation of heat and power. Will include (i) formulating a quantitative description of energy demand and as a function of utilization temperature for the US, (ii) evaluation of power cycle and district heating design options and opportunities for a range of scales from distributed use in buildings and communities to central station applications in the Northeast region, (iii) economic analysis with tradeoffs included for well drilling costs as a function of depth to increase production temperatures and plant performance

Computational Design of New Low-k dielectric Materials for Next-Generation Computers (Paulette Clancy)

Project Summary: I am looking for 1 or 2 students to use a software package, TINKER, for the virtual design of materials for the next generation of semiconductor materials for interconnects. TINKER includes a Molecular Dynamics simulation code which essentially solves the equation, $F=ma$, as time evolves.

We want to explore **a new route to more robust low-k materials through sub-microsecond laser annealing using a novel computational approach** as a precursor to complementary experiments. We avoid undirected trial-and-error searches of the broad parameter space that exists for experimental laser annealing studies using realistic molecular-scale models and appropriate computational approaches to predict likely outcomes for ultra-fast laser annealing strategies for existing low-k spin-on materials. These studies provide a vital first step towards a fundamental understanding of the link between annealing conditions and the electrical/mechanical behavior of porous low-k materials that could point the way to the design of better performing materials.

As the figure shows, the lower the dielectric constant, k, the worse Young's modulus becomes. We are interested in using materials with a k value of about 2.0, but finessing the poor mechanical properties through laser annealing.

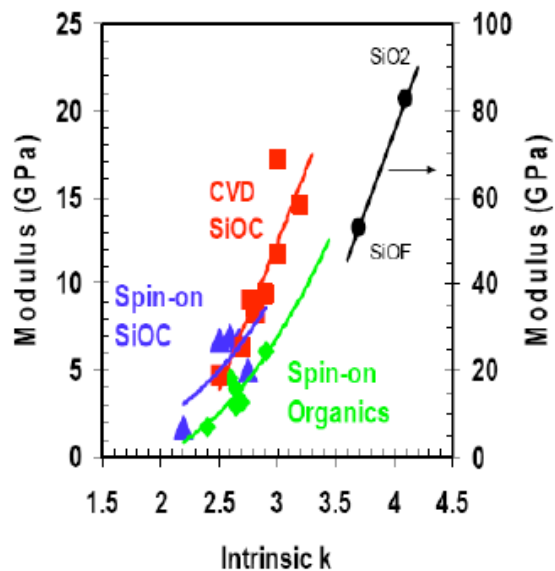
In 2006, laser spike annealing demonstrated factors of 3-5 improvement in Young's modulus with only minimal (10%) increases in the dielectric constant, including films with dielectric constants below 2.0. This is an extremely promising result, but it is far from a production-level success: The nature of the structural changes which occur in these $>1000^{\circ}\text{C}$ anneals is largely unknown and raise fundamental questions about the design of "ideal" porous structures in this environment.

Semiconductor Research Fellowship Support:
A \$5,000 Fellowship will be provided to up to two students working on this project.

Prior Computational Experience: This project will be awarded to the student(s) with a strong interest in and some demonstrated skill in computational work.

Specific Tasks: The M.Eng. student (or students) working on this project will be concerned with the following tasks.

Task 1: Produce virtual SiOC(H) samples. We will improve the selection process adopted by



Tajima (1-3] to create structural ‘samples’ representative of real amorphous SiOC(H) polymers: They employed no statistical methodologies to determine if the physical properties of the sample were sensitive to the type of candidate structure chosen, nor how well the properties might be improved by different sampling. We intend to investigate this systematically. Tajima’s group also did not test the sensitivity of their results to changes in intermolecular potential models. This deficiency could be serious: even simple molecules can be predicted to be planar (Brenner model), curved (MM3 model), or be significantly twisted out of plane (DFT), depending on the potential used to model it. We will test the veracity of selected models to reproduce existing experimental equilibrium data and Kroll’s DFT structures for known SiOC(H) candidate materials [4].

Task 2: Predictive studies of laser-annealed SiOC(H) systems. Samples of candidate low-*k* materials produced in Task 1 will be subjected to ultra-fast heating within a Molecular Dynamics simulation that emulates the experimental process and then follows the ultra-fast cooling that results when the heating stops. We will follow the time evolution of candidate material systems during and following laser treatment, looking at structural and property changes that occur as laser annealing conditions (pulse duration and intensity, for instance) are varied. We will also use Molecular Dynamics to calculate Young’s modulus of the resultant material. We will calculate the equilibrium properties of candidate low-*k* materials and use the data to understand (and decouple) how strain and carbon content affect the material’s mechanical strength and their response to laser annealing.

Student’s background: We can teach any M.Eng. student to use the code but we would prefer a student with some experience or propensity for computational work. The grad student mentor for this project is a senior PhD student,. [Note: No knowledge of molecular computer simulation is expected.]

References

1. N. Tajima, T. Ohno, T. Hamada, K. Yoneda and N. Kobayashi, S. Hasaka and M. Inoue, Molecular modeling of low-*k* films of carbon-doped silicon oxides for theoretical investigations of the mechanical and dielectric properties, *Appl. Phys. Lett.*, 89, 61907 (2006)
2. J. Ushio, T. Hamada, T. Ohno, S-I Nakao, K. Yoneda, M. Kato, N. Kobayashi, Structures and Properties of an Ultra-Low-*k* Material: Classical-molecular-dynamics and First-principles Calculations, *MRS Symp Proc.*, 914, 21-26 (2006)
3. N.Tajima, T. Ohno, T. Hamada, K. Yoneda, S. Kondo, N. Kobayashi, M. Shinriki, Y. Inaishi, K. Miyazawa, K. Sakota, S. Hasaka, and M. Inoue, Carbon-Doped Silicon Oxide Films with Hydrocarbon Network Bonds for Low-*k* Dielectrics: Theoretical Investigations, *Jpn. J. Appl. Phys.*, 46, 5970-5974 (2007)
4. P. Kroll, Modelling and simulation of amorphous silicon oxycarbide, *J. Mater. Chem.*, 13, 1657 (2003)

Virtual Design of Organic Materials to Capture Carbon (Paulette Clancy)

Project Summary: My group and I looking for 1 or 2 students to use a freeware software package, TINKER, for the virtual design of materials to capture carbon dioxide from waste streams. TINKER includes a Molecular Dynamics simulation code which essentially solves the equation, $F=ma$, as time evolves.

A new class of organic materials called NIMs (nanoscale ionic materials) and NOHMs (nanoscale non-ionic materials) was discovered at Cornell (by Archer and Gianellis) and are under investigation as a way to capture CO₂ from waste streams. Our computational project involves designing NIMs or, more likely, NOHMs tethered to a surface that optimize the capture of CO₂ molecules and then, preferably by temperature “swing”, allow the carbon dioxide to be recaptured for storage. Our goal is to design NOHMs that make carbon capture easy.

Prior Computational Experience Needed: None

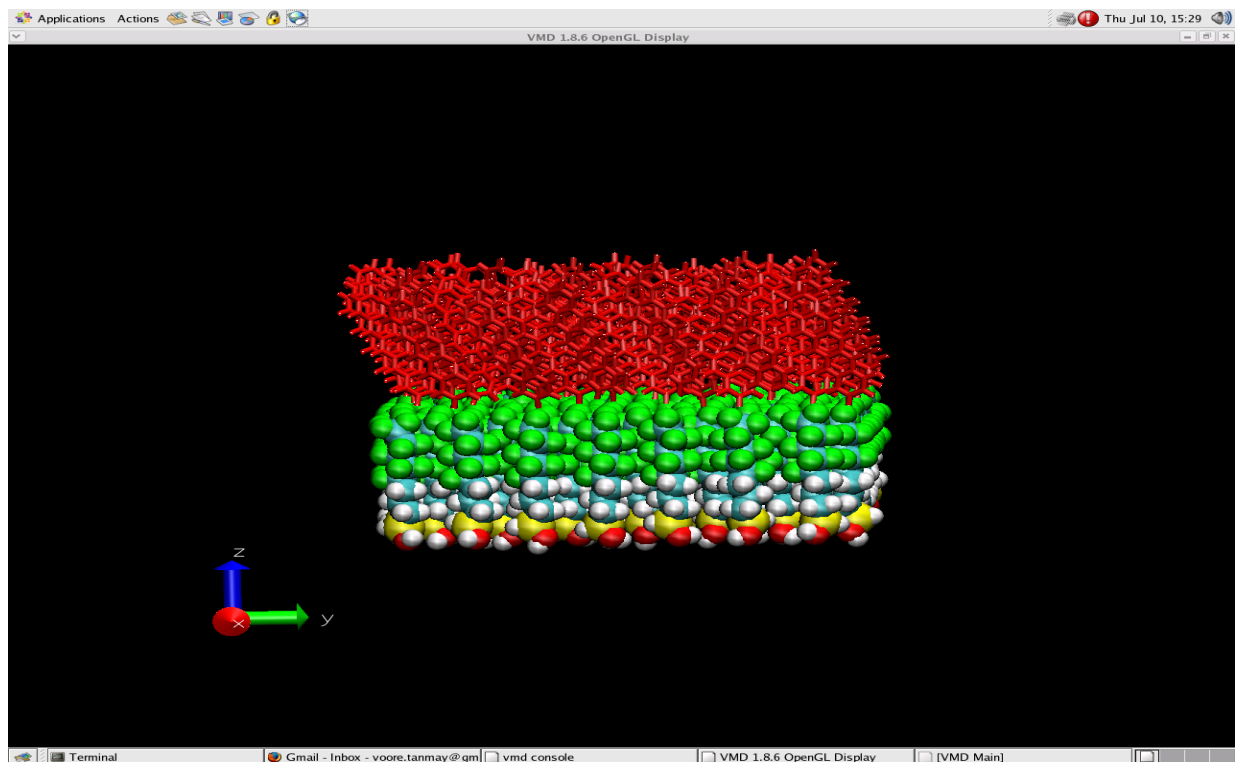
Project Status: Our work on a related project on solar cells that involves self-assembled monolayers has shown that molecular simulation is able to view (through movies) the process by which small molecules are trapped by the waving motion of long-chain self-assembled alkyl molecules (see Figure 1 below). In that case (for semiconductor molecules) it was undesirable to have molecules insert between the SAM molecules. But for carbon capture, it will be desirable for CO₂ to intersperse itself among the alkyl chains constituting the SAM. We plan to predict the physical conditions under which CO₂ insertion (capture) is maximized and then investigate how easy it is to release the trapped CO₂ when you are ready to store it safely.

If results look promising, we will test our predictions against experimental data through a collaboration with Prof. Alissa Park (ChE/Columbia).

Specific Task: The student (or students) working on this project will vary parameters such as the density of the SAM and the chemistry of the SAM molecules to see the effect on the sticking coefficient for different SAM molecules (C7-C8 and C11- and C-12 alkyl chains).

Student's background: We can teach any student to use the code (this summer we taught an undergraduate student to start getting results within a week). The grad student mentor, a senior PhD student, has lots of experience helping undergraduates to quickly ramp up to speed. [Note: No knowledge of computer simulation is expected and no programming or code development is involved in this project.]

Figure 1: Monolayer of the organic semiconductor, pentacene (red wire frame objects), adsorbed on a self-assembled monolayer, a C8-alkyl chain (filled atoms) with fluorine termination (green atoms) on an oxide surface (not shown).



Vibro-Wind Project: Experimental Devices for Energy Scavenging using Small Wind Currents (Paulette Clancy)

Project Summary: A multi-disciplinary group of faculty (Professors Mike Thompson [MSE], Wolfgang Sachse [TAM/MAE], and I) in the College of looking is looking for one or two M.Eng. students to help fabricate electronic devices in CNF (Cornell Nanofab Facility) that will scavenge the energy produced when millions of tiny *cm*-scale steel fingers (cantilevers) oscillate in the breeze, for example, envision these diode devices as a “hairy” coating on buildings that collects the vibrational motion caused by the wind and turns it into DC current.

This so-called “vibro-wind power” harvests power generated by wind flowing over and vibrating an array of piezoelectric fingers. Each finger or element has a piezoelectric material deposited on a stainless steel substrate. The diode is deposited on top of the piezoelectric layer, as shown in the top and cross section views below. The purpose of our experiments is twofold. The first goal is to optimize the diode surface area for use on the piezoelectric vibro-wind elements. The second goal is to conduct a feasibility study of using a stainless steel substrate for the piezoelectric element.

Prior Experience Needed: None. You will be trained at CNF to emulate these tasks and create what are called Schottky diodes.

Project Status and Proposed Tasks for AY 09-10:

The ultimate practical implementation of these devices, if they show sufficient promise as “energy scavengers,” will probably need stainless foils for toughness, as much as cost and conductivity. Thin polished stainless steel foil is readily available due to developments in solar cell and flexible display applications. Cutting and working with such foils in the CNF requires some effort, but is a phase for later in the project.

Initially though, our prototype device is being developed on silicon, rather than SS foils, for which the CNF is very well suited. The first step is development and characterization of the Schottky diode on a doped (or undoped) silicon substrate. Subsequent steps will establish and validate a process for the full device stack; this can (and probably should) be done on Si wafers first.

To get reasonable deflections and frequencies, the cantilevers need to have specific dimensions. The target frequency is 10 Hz with as large deflections as possible. In parallel with the diode fabrication, a design could proceed based on a cantilever design, perhaps using thin Si wafers if the ideal thickness is in the >50 um thickness, The conductivity of Si will be adequate for the amount of charge we are discussing, but fracture toughness will always be an issue.

The goals this year are to create working diodes, optimize the dimensions of the cantilever Si thin film, and measure the current produced. Then create a process to make arrays containing hundreds of these cantilevers as the first step to demonstrating the viability of this exciting project.

**Prospects of Massive Investment in
Resid Desulfurization within Ten Years
(Andrew Hunter)**

Background. Prof Phil Verleger wrote in 2006 that oil prices would rise to \$100 because environmental regulations were coming in conflict with global crude supplies. In particular, he noted that the Europeans were demanding that almost all sulfur be removed from diesel as the US had. He suggested that refiners lacked sufficient capacity to remove sulfur from crude. Their response, he suggested, would be to bid up the price of sweet crudes. He also suggested that OPEC nations would cut crude production rather than allow the differential between light and heavy crude to become large. He believes he was right and, further, that the IEA endorsed his view in their Medium Term Outlook, issued June 30th 2009.

Possible scenarios. The world desulfurization capacity has been relatively static in the last year and so there is a good chance of a replay of the 2008 price rise as Asian economies recover, if Prof Verleger is correct. One way to counter this would be to rapidly add capacity to desulfurize

the products of sour, heavy crudes in those areas such as Asia where the growth is occurring and where refineries are less complex than in the US, Europe or Japan.

Added to this concern is the fact that authorities in the US are considering a requirement that oil products meet increasingly strict limits of contaminants such as sulfur. New York City aims to reduce the sulfur limit on fuel oil, currently 0.3%, or 300 ppm, to below 15 ppm.

Questions raised. As most publicly available projections for world crude demand show a steady increase above its current level, it is likely that both of these pressures will get greater. This raises the technical question of which route to lower sulfur is best given that there are limits to the output sulfur level from catalytic desulfurizers of heavy resids. In some parts of the world, there could also be a shortage of natural gas from which to source hydrogen at a reasonable cost. An alternative to resid desulfurization would be coking, followed by desulfurization of the lighter gasoils and burning the coke to make electricity. This project would examine these questions.

Project plan:

- Step 1: review literature on the desulfurization of heavy resids and heavy coker gasoils.
- Step 2: develop algorithms from the best available rate or space velocity data.
- Step 3: examine the effect of metals on reactor operations and product qualities.
- Step 4: review current limiting specifications for heavy oils and make a considered projection of where these specifications will be in the next 5-10 years.
- Step 5: simulate a 50,000 barrel per day reactor for Saudi heavy vacuum resid.
- Step 6: develop a ranking methodology for the set of worldwide crudes, ordering them by difficulty with which their resids can refined to meet specifications.
- Step 7: examine disposition of refining capacity in Asia, Europe, Japan the Americas
- Step 8: relate availability of natural gas to potential sites for treating heavy, sour crudes.
- Step 9: estimate the cost of building treating facilities for heavy, sour crudes
- Step 10: issue report

Timing, in weeks:

Step 1	lit review	6
Step 2	algorithms	4
Step 3	metals	3
Step 4	specifications	4
Step 5	simulation	6
Step 6	ranking	6
Step 7	disposition	6
Step 8	natural gas	6
Step 9	cost	6
Total		47

Using Wind and Solar Farms to Recover Water in Arid Regions (Andrew Hunter)

Problem. Large parts of the world have little water but may have the conditions needed for considerable supply of energy from wind.

Project. Where are these areas, where would the water come from and what turbine and solar design would be appropriate, taking into account that the regions with wind might lack regular and proficient maintenance? The results should come together in plant design and costing.

The project should consider using sea water, sewage and water condensed from the atmosphere. It would liase with “Potable Water Recovery from Humid Air” (AI Center). It is a task suitable for a team of 2-4 people and will take 1 semester. It may produce answers that lead to a second semester’s work in the Spring.

Reference. <http://www.technologyreview.com/energy/17862/>

Nanotechnology Coatings (AI Center)

Company. A local startup company, iFyber, is focused on nanotechnology coatings of textiles for high tech applications. The company has patent pending proprietary technology and is scaling up its processes.

Project Description. The goal of this project is to develop a laboratory scale process for this novel technology. This laboratory scale process will be used to develop predictive data for further industrial scale up. The Master of Engineering candidate will work under the direction of the company’s technical team to develop data using multivariable analysis techniques including Design of Experiment approaches on laboratory scale equipment.

Timing. The company seeks to have its first lab scale process design in place by the end of October 2009.

Requirements. This project is a combination of experimental and analytical/design activities. The candidate must be comfortable in a laboratory setting and be able to transition from theory to practice. The ideal candidate for this project should have the following skills:

- Self motivated.
- Works well in a team environment.
- Interest in hands-on problem solving.
- Good laboratory technique
- Knowledge of multivariable analysis or ability to quickly learn statistical techniques.
- Good knowledge of basic chemical engineering unit operations.
- Good communication skills.

Throughput Monoclonal Antibody Formulation and Stabilization (David Putnam)

Most monoclonal antibodies are administered intravenously over long timeframes. A number of pharmaceutical companies would like to administer monoclonal antibodies subcutaneously so that patients can self-administer their antibody medications at home, much like insulin is administered today. The problem is that to reduce the injection volumes of the antibodies, the proteins must be formulated at very high concentrations. Because the kinetics of antibody aggregation is a function of concentration, a formulation goal of ~100mg antibody/mL is very challenging. The focus of this project is to use combinatorial, high throughput formulation methods to discover new antibody formulations with the capability of stabilizing monoclonal antibodies at high concentrations. The investigators will not only learn the principles of protein formulation, but also will become experts in robotic liquid handling and the analysis of proteins (dynamic light scattering and SDS page protein gel analysis).

A Breakthrough Sustainable Energy System (David Putnam)

Heat generation systems suffer from poor energy/heat conversion yields. This project focuses on the development of a prototype system that approaches 100% conversion yields, potentially leading to a system that can sustain hundreds of degrees Celsius with very low energy input. The application of the prototype is potentially extensive. The research team will learn engineering principles of heat transfer and physical principles of electromagnetic radiation and its application to molecular vibration heating. The resulting prototype, to be built by the research team will serve as the potential basis for a new sustainable energy company.

Cerebral Blood Flow in Polycythemia Vera (William Olbricht and Chris Schaffer)

Polycythemia vera (PV) is a disorder in which a genetic mutation stimulates bone marrow to overproduce red blood cells. The elevated hematocrit (red cell volume fraction) in PV leads to a variety of clinical symptoms, including thrombosis and stroke. These symptoms are manifestations of abnormal blood rheology and altered interactions between blood cells and the vascular endothelium owing to the elevated hematocrit.

Our collaborators at the Weill Cornell Medical Center, Dr. Richard Silver and Dr. Andrew Schaffer, have compiled an extensive database of PV patient therapies and outcomes. However, it is difficult to make connections between patient characteristics, histories, and symptoms and the underlying mechanisms of the disease. Therefore, the goal of this project is to understand the relationship between blood flow alterations and PV symptoms. We focus on blood flow in the

brain, because PV patients often exhibit diminished cerebral blood flow, which can be responsible for some of the most critical complications of PV.

Professor Chris Schaffer's lab uses two-photon microscopy to study *non-invasively* red cell motion in individual blood vessels in the brain. They have gathered data on the distribution of red cells among blood vessels and the flow rates in individual blood vessels for rats with elevated hematocrit. The data are especially robust for an *in vivo* experiment, because they give details of the vessel network architecture and flow changes in individual vessels. However, interpreting the data is challenging, and it could be greatly enhanced by having a quantitative model that can simulate the experiments and help interpret the results.

The goal of this project will be to build a computational model based on well-known principles of mass and momentum conservation applied to each vessel. These conservation laws will be reduced to a system of relatively simple equations that can be solved numerically using standard techniques to determine time-dependent flow rates, pressures, cell density, and cell velocities throughout a network of blood vessels. The velocity, cell density, and pressure may be functions of time, and the computational tool will track the time dependence of these variables.

The computational tool will be applied to specific experiments that have been done in the lab to compare predicted results with experimental data. For example, preliminary data show that when the hematocrit exceeds its normal value, an unusually high number of capillaries exhibit sluggish flow with very low red cell velocities inside the vessels. We will use our model to simulate this experiment, and use the results to extrapolate to higher hematocrit values that have not yet been achieved experimentally. Many such "numerical experiments" can be imagined to help expose the origin of some of PV's clinical symptoms. Ultimately, we intend to use the microscale model to help interpret patient data compiled at WCMC.

Some expertise in fluid mechanics is helpful, but not a requirement for the project. The equations are easy to formulate, and their implementation in this problem does not require extensive training in fluid mechanics.

High-Frequency Ventilation for Neonates (William Olbricht and William Frayer)

Premature infants often require mechanically assisted breathing during the first few weeks of life while their lungs develop completely. In some patients, special breathing machines are used to provide high-frequency ventilation (HFV). HFV delivers small bursts of air at very high frequencies – much higher than normal breathing rates. HFV has proven effective in delivering oxygen to neonates when conventional mechanical ventilation is inadequate. Despite its widespread use, HFV can be difficult to control in clinical practice. Parameters such as pressure, air volume, and ventilation frequency are set based on heuristic rules that rely on physicians' experience and intuition.

This project involves using a computer model to predict and assess the performance of HFV in realistic situations. The model uses computational fluid dynamics to determine the motion of gases in an infant's airways under HFV. Results from the model will be correlated with macroscopic parameters that are observed and recorded during HFV in the clinic. Previous M.Eng. teams started the model development; the current project involves continuing development, refinement, and correlation with data. This project is suitable for an interdisciplinary team of students. The project will be carried out in collaboration with Dr. William Frayer in the Neonatal Intensive Care Unit at Weill Cornell Medical Center.

Medical and Industrial Biotechnology
(Matt Delisa and Jeff Varner)

Projects for students participating the Medical and Industrial Biotechnology (MIB) specialization will originate from the MIB laboratory. The MIB laboratory in the fall semester covers a variety of techniques including recombinant DNA and cloning, cell culture, protein production, small- and large-scale separations, and bioreactor design and operation. The design project in the spring semester applies methods and techniques learned in MIB Laboratory to a faculty-mentored independent project. Students investigate candidate projects in the fall semester under the auspices of CHEME 5450 (Bioengineering Logic and Design). After choosing a project, each student produces a prospectus containing a problem statement, significance, plan, and timeline for proposed project. Work on the project will take place in the spring semester.

Students not participating in the MIB specialization may still be interested in an M.Eng. project in the general areas covered in the MIB program. In this case, student should contact Professor Delisa and Varner to explore possible projects.