POSSIBLE SC476 CAPSTONE PROJECTS – CLASS OF 2008

(1) DEVELOPMENT OF FORENSIC TOOLS FOR SMOKE RESIDUE AND DEPOSITION ANALYSIS

Current forensic methods in fire investigation do not make use of the potentially rich information available in smoke deposited on surfaces. While smoke deposition pattern analysis is included in standard fire scene patterns analysis, the chemistry and physics of smoke deposition is poorly understood. Even more significantly, analytical chemistry methods have not been widely used in the interpretation of smoke deposits. This type of analysis has the potential to identify the presence of accelerants, to identify the fuels burned during the ensuing fire, and to identify the combustion mode(s) and temperatures under which the smoke was produced and deposited. The objective of this project is to develop methods and scientific bases for the use of smoke deposition analysis as a forensic tool. This work is being carried out under a Department of Justice grant. Samples will be provided by a local Fire protection engineering firm (possible field trip to see samples generated). The analytical tools that can be applied to the samples include IR and Raman spectroscopy, GC-MS, TGA, TGA-MS, DSC, AFM, SEM, solvent extraction, and MALDI. Several groups can work on this project if they choose different techniques to explore.

(2) STUDIES OF THE IMPACT RESISTANCE OF POLYMER-COATED METALS

Protecting military personnel from the effects of mines, bombs, improvised explosive devices (IEDs), and small arms fire is an area of great interest to the military particularly in this era of ground-level warfare. Recent studies of polymer-coated armor have revealed enhanced protective properties over the bare metal. Humvees with a polymeric spray-on coating were demonstrated to protect the occupants inside against explosions and shrapnel. While many of these studies have documented the enhanced protective properties of various polymer-based coatings, the mechanism of this protection is generally unknown. The goal of this research is to investigate on a fundamental level the relationship between polymer properties and impact resistance. Why do polymer coatings enhance the impact resistance of metal substrates? How can polymer coatings be tailored to provide high performance against multiple threats and under a range of environmental conditions? For this capstone project, laboratory-scale tests of the impact resistance of various polymer coatings will be conducted. One coating will involve model networks of polydimethylsiloxane (PDMS) of varying crosslink densities (as synthesized in IL4). How does crosslink density affect the impact resistance of the coating? Another coating will involve polyvinylacetate (PVA) which has a glass transition temperature slightly above room temperature. Since polymer properties change with temperature, particularly around the glass transition, impact properties of PVA-coated metal will be measured at various temperatures. Students will synthesize or prepare the polymer coatings and use a laboratory-scale impact testing device (modified air rifle) to measure impact resistance.

(3) FUEL ANALYSIS AND CHARACTERIZATION STUDIES

(in collaboration with the Mechanical Engineering Department)

(A) Fischer-Tropsch Synthetic Diesel Fuel Characterization

The USNA Mech E Dept. is engine testing a new synthetic diesel fuel created from a Fischer Tropsch Process. It is believed that the fuel is principally straight chain paraffin, nominally with 16 carbons. In order to understand engine performance better we are interested in a fuels characterization of this synthetic diesel fuel. A comparison to base diesel fuel with its characteristically high aromatic and sulfur content will be of interest.

Project deliverables are seen as a determination of the carbon number of the various paraffins within the fuel, the mass fractions of each major carbon group, a comparison of the sulfur content of baseline diesel and Fischer Tropsch fuels, error analysis and a summary of lessons learned during the characterization process and recommendations (if any) for additional characterization techniques.

(B) Diesel Soot Metal Content

The USNA Mech E Dept. is testing alternative diesel fuels. We are interested in analysis of diesel engine exhaust soot for trace metal components. This project will likely involve testing of base fuel and oil samples also to see if the metal in the soot may be fuel, oil or possible engine structure derived.

Project deliverables are seen as a determination of the various metals within the fuel and lubrication oil along with characterization of any metals in the soot, the mass fractions of each metal found, and a comparison of the metal content of baseline fuel and lubrication oil to that of metals found in the soot. Error analysis of the results should be attempted. A summary of lessons learned during the characterization process and recommendations (if any) for additional characterization techniques would be useful for future analysis attempts.

(C) Diesel Soot Soluble Organic Fraction (SOF) Analysis

The USNA Mech E Dept. is testing alternative diesel fuels (Fischer Tropsch Synthetic Diesel and Bio-Diesel). Data regarding SOF from diesel engine soot will be very useful in understanding new alternative diesel fuel performance. Deliverables should consist of the characterization of SOF found in exhaust soot along with the nature and composition of the SOF fraction within the soot. These analytical results should have an error analysis performed. A summary of lessons learned during the characterization process and recommendations (if any) for additional characterization techniques would be useful for future analysis attempts.

(D) Effect of lubricating oil dilution from alternative fuels

The USNA Mech E Dept is testing alternative fuels such as biodiesel and Fischer-Tropsch diesel for use in fleet engines. During normal engine operation, some unburned fuel accumulates in the engine crankcase and dilutes the lubricating oil. We are interested in the effects of dissolved fuel on lubricating oil. This project would likely be shared between students from both the Chemistry and Mechanical Engineering depts. From a chemical perspective, how does the composition of various fuel/oil blends change over time or as a function of heating? Are the blends chemically stable? Mechanically, how is oil lubricity and viscosity affected by fuel intrusion? Do these performance properties change over time? Are there safe limits for fuel contamination percentage? Is this fleet testable? Does mixing these fuels with oil make water absorption more of a problem (compared to standard diesel)? Are there alternative oils available that may more

resistant to contamination? Project deliverables may include heating and aging effects data, performance data and recommendations for testing standards that may be applicable for fleet operation. Error analysis and a summary of lessons learned during the characterization process and recommendations (if any) for additional characterization techniques would be useful for future analysis attempts.

The Mechanical Engineering Department will provide fuel, lubricating oil and soot samples.

(4) COMPARISON OF TECHNIQUES FOR STANDARDIZING PEROXIDE SOLUTIONS

Hydrogen peroxide is used as a disinfectant and to brighten teeth. This molecule is also fairly ubiquitous in the environment. Accurate determination of the concentration of peroxides touches many fields from food chemistry to rocket fuel. This project involves examining several approaches for standardizing hydrogen peroxide and short chain organic peroxide solutions. The project will begin with an examination of the literature and traditional approaches to standardization of hydrogen peroxide solutions. The students will compare several titrimetric methods, for example $KMnO_4$, Ce(IV), and iodimetric methods. The project will also compare the accuracy and precision of end point determination by spectroscopy or visual endpoint. The best technique for standardizing organic peroxide solutions will be determined.

(5) INVESTIGATION OF FACTORS AFFECTING ENZYME ACTIVITY AND STABILITY

The activity of the enzyme staphylococcal nuclease will be studied by measuring the activity in the presence of different substrates and inhibitors using a spectrophotometric assay. The reaction conditions will also be varied with respect to temperature, buffer pH, and presence of specific denaturing agents such as urea, guanidine, and lauryl sulfate. The stability of the enzyme will be determined under various conditions by monitoring the spectroscopic signature (fluorescence and ultraviolet) of the protein as it is incrementally denatured. Protease accessibility, a measure of the compactness of the folded state of the protein, will be assessed by MALDI-TOF mass spectrometry. The enzyme was isolated by previous capstone students and is ready for use in these studies.

(6) DETERMINATION OF CAPSAICIN IN HOT PEPPERS

Hot peppers, also known as chili peppers, are a group of species in the genus *Capsicum* of the potato and tomato family. The chemicals responsible for the heat (pungency) in chili peppers, and hence hot sauces, belong to a class of compounds known as capsaicinoids. Capsaicin and dihydrocapsaicin are responsible for over 90% of the heat in hot peppers. Other capsaicinoids are present in trace amounts and also contribute to the heat. In this project, the students will investigate the origin of the Scoville scale and conduct the original Scoville tests (human taste tests of the “hotness” of peppers). The students will then develop an analytical method (HPLC)

to determine the amount of capsaicin in the peppers and compare the results to those of the Scoville tests. Various hot sauces can also be tested and compared to the natural peppers.

(7) MATERIALS AND SOLID STATE CHEMISTRY: SYNTHESIS AND CHARACTERIZATION

Solid materials can have exceptionally interesting catalytic, electronic, and optical properties. In this project, students will synthesize high temperature superconductors (1-2-3 compounds) using various methods and compare the properties of their products. Is the product a superconductor? Other properties will be measured via SEM or X-ray diffraction. The coordination numbers and coordination geometry of all the metal cations in the superconductor can be determined.

(8) LABORATORY DEVELOPMENT FOR IL2

In Integrated Laboratory II, a multistep synthesis is attempted. Currently the syntheses attempted are chosen for ease of synthesis and sometimes students have commented that there did not seem to be a purpose for synthesizing the molecules chosen. This project involves developing a new type of multistep synthesis with target compounds with a clear purpose. For example, sunscreens are a common commercial product. Sunscreen consists of compounds which absorb UV light, suspended in a cream base. The midshipmen undertaking this project would need to conduct a literature search to determine what compounds are used in these products and to see how the compounds are synthesized. Once the synthetic routes are known, the midshipmen would adapt the route for use in an undergraduate setting, including finding appropriate characterization methods such as IR and NMR spectroscopy. They would also then examine methods for measuring the light absorbing characteristics of the compounds. This would be to see if the compound is suitable for use at blocking UVA or UVB light. The thrust is to develop a laboratory that would involve a challenging but achievable synthesis and also include an analytical chemistry component.

(9) LABORATORY DEVELOPMENT PROJECT

The midshipmen will improve a current Integrated Laboratory (IL) experiment or develop a new IL experiment that would be of interest to students. The experiment must support concepts and techniques used in the IL courses, and feasible for use in a student laboratory. Instructor approval is required before the start of the semester.

(10) STUDENT DESIGNED PROJECT

The midshipmen will design their own chemistry project. Instructor approval is required before the start of the semester.