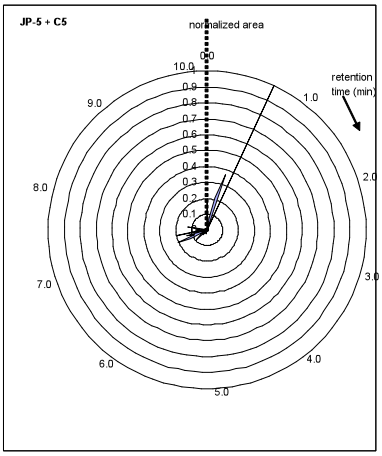
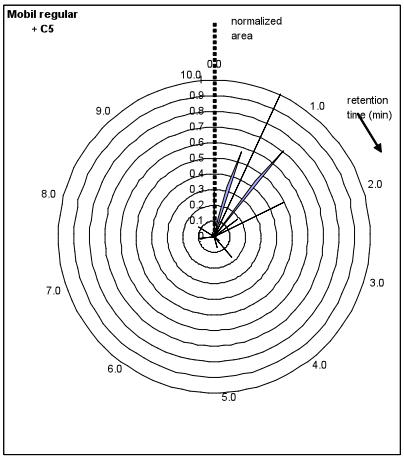
# SC476 CAPSTONE PROJECTS – CLASS OF 2010

## EVALUATING THE "zNOSE™" PICTOGRAM METHOD FOR IDENTIFICATION AND DIFFERENTIATION OF FUELS AND LUBRICANTS

Common fuels and lubricants are complicated hydrocarbon mixtures that may consist of dozens of compounds. They can be completely characterized by analytical techniques, such as GC, which separate and quantify each of the components. Direct comparison of the chromatograms permits identification of a specific sample with the refinery or distributor batch, or allows differentiation of different types of fuels. This type of comparative analysis is extremely useful in many areas, including quality control and forensic investigations, but the actual comparison can be quite tedious. A new sensor device, the "zNose™", is an electronic odor sensor that is based on GC analysis, but also offers a novel way to characterize the odor qualitatively, in a pictogram. (See "The zNose" by E.J. Staples, *Sensors Magazine*, June 2001.) By making a polar plot of component concentration vs. retention time, a visual image of the odor is created. These olfactory images can be readily compared by anyone, even people without technical expertise. In essence, the chromatogram provides a view of the individual "trees", while the pictogram is like looking at the forest as a whole. Sometimes a view of the forest is all that is required. The purpose of this project is to evaluate the potential of such pictograms for the identification and differentiation of various fuels and lubricants. The illustration suggests that distinguishing between JP-5 (on the left) and regular unleaded gasoline is readily done by the pictogram method. Is that a general finding? Is it possible to use pictograms to, for example, tell the relative octane level of the fuel? Can it distinguish different brands of fuel, at the same octane level? Can it identify one sample with a specific gas station? Can it identify fuels treated with ethanol or oxygenating agents? Similar questions can be asked about lubricating fluids as well. The utility of the method will be easily tested - if the viewer can identify characteristics of a fuel simply by visual comparison of an unmarked pictogram with those of know "standards", then the method has validity.



## MICROWAVE SYNTHESIS OF ORGANIC COMPOUNDS

In your Organic Chemistry course, you used many methods for preparing organic compounds, including simple heating, the use of catalysts, etc. In recent years, the use of microwave reactors has been explored as a simple yet effective way to increase the reaction rates of various reactions, sometimes without even using a solvent! This project involves running some typical organic reactions in a microwave reactor, changing conditions such as reaction time and temperature. Some microwave-assisted reactions take only a few minutes, so there is ample opportunity to explore these variables. Product workup will be carried out by the usual chromatographic techniques (GC, GC-MS, LC). Some suggested reactions are $S_N2$ reactions (amines reacting with chloroalkanes), particularly as applied to the synthesis of ionic liquids. Other possibilities include microwave-assisted rearrangements (Fries rearrangement), Friedel-Crafts, or other reactions under solvent-free conditions, in standard organic solvents, or in ionic liquids. This project is a good way to become better acquainted with organic chemistry and to understand the possibilities of a new technique to accelerate organic reactions.

## FUEL ANALYSIS AND CHARACTERIZATION STUDIES

(In collaboration with the Mechanical Engineering Department)

### 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.

The Mechanical Engineering Department will provide fuel and soot samples.

## MATERIALS AND SOLID STATE CHEMISTRY: SYNTHESIS AND CHARACTERIZATION

Solid state materials can have exceptionally interesting catalytic, electronic and optical properties. In this project students will synthesize a number of materials including high temperature superconductors, layered metal disulfides, and mesoporous silicas. The superconductor will be made by combination of low temperature preparation, then high temperature firing. The layered metal disulfide will be made using high temperature vapor transport in sealed tubes. Intercalation reactions will be performed on the resulting crystals. Mesoporous silicas will be made using decomposition onto a large molecule template. Characterization of these materials will use a variety of techniques including X-ray diffraction, X-ray fluorescence, thermogravimetric analysis, scanning electron microscopy and electronic measurements.

## TRACE METAL CONCENTRATIONS IN USNA DRINKING WATER USING ICP-MS

Metals in drinking water are a major concern to human health. Lead can cause damage to the brain, kidneys and the functioning of red blood cells. Changes in the treatment of drinking water in the DC area resulted in the release of lead from the distribution system (http://www.epa.gov/dclead/). The lead was in the pipes and its release resulted in concentrations of lead that were above EPA's 15 ug/L action level causing concern among the residents and action by the water district to correct the problem. This project will measure metal concentrations in the drinking water at the USNA using inductively coupled plasma – mass spectrometry (ICP-MS). An ICP-MS instrument has recently been acquired by the Chemistry Department and it has the capability for multi-element analysis with a relatively short analysis time (less than a few minutes per sample). The project will involve: 1) development of an analytical method for metals using ICP-MS, 2) development of a trace-metal clean sampling methodologies, and 3) sampling strategy (e.g. how many and how often do samples need to be collected to answer a specific question). One possible question to investigate is if there is any leaching of metals within the distribution system at the USNA.

## GREEN CHEMISTRY AND RED TOMATOES

Lycopene is an antioxidant with several studies suggesting diets of lycopene-rich foods can provide health benefits. It is a carotenoid pigment that gives tomatoes, grapefruit, and watermelon their red color, with tomatoes having the highest lycopene content. Pure lycopene is quite expensive (~$2400 per kilo in pure form) but every season farmers dispose of massive amounts of overripe or blemished tomatoes which do not meet USDA quality standards. Could these be a cheap source of this powerful antioxidant? In the project, students will be comparing two extraction methods: a traditional organic solvent-based extraction and a solvent-free emulsion extraction. Which method is more efficient in extracting lycopene? Which is "greener" with respect to the 12 principles of green chemistry? Does a red tomato have more lycopene than a green one?

## CONSTRUCTION AND EVALUATION OF A SIMPLE SPECTROMETER

Many of the instruments we use in the instructional program are commercial instruments which, while very capable, do not give a real feel for the parameters being measured. This project involves the construction of a very simple spectrometer (colorimeter ) using LEDs as light sources and a photocell (CdS or other device) as detector. Such a system is ideal for presenting the basic principles of spectrophotometric measurements, and it may find later use in the IL or plebe chemistry sequence. A prototype has already been prepared as a demo for IL2, but much more work needs to be done to get quantitative results for real-world samples. This system is battery powered, and the detector circuitry is very simple, so only a basic knowledge of EE is required! The initial system can be quickly constructed from PVC pipe and some LEDs to choose the wavelength, followed by evaluation of Beer's Law with solutions absorbing in the visible region. Common applications can then be explored, such as iron or phosphate determinations. Another possibility is fluorescence measurements by monitoring the light beam at right angles to the LED beam. Comparison could then be made to the riboflavin determination you did in IL2 using a commercial instrument.

## 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.

## STUDENT DESIGNED PROJECT

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