CHE 451, Chemical Engineering Design II, is described in the NCSU course catalog as:

“Chemical process design and optimization. The interplay of economic and technical factors in process development, site selection, project design, and production management. Comprehensive design problems.”

“Comprehensive” is an understatement. The course challenges students with a wide variety of chemical engineering processes, ranging from the production of beta-lactam antibiotics to biodiesel. Other teams have designed products including a microfluidic device for the detection of V. cholerae in drinking water and a miniature UV-NIR spectroscopy apparatus to detect chemical warfare agents. In addition, students complement their technical skills with teaming, leadership, project management, and communication skills. Both the instructors and the students feel an enormous sense of pride as we view the accomplishments of almost seven months’ work.

We wish to thank those individuals and companies who have sponsored and advised projects this semester. The task of coaching 20 teams consisting of 70 students from three different academic departments and three colleges could not have been accomplished without your help!

Mr. Jeff Brown (Wyeth Vaccines)
Mr. Severin Butler (Biogen-Idec)
Dr. Med Byrd (NCSU Department of Paper Science and Engineering)
Dr. Chris Daubert (NCSU Department of Food Science)
Dr. Peter Fedkiw (NCSU Department of Chemical and Biomolecular Engineering)
Dr. Juan Hinestroza (NCSU Department of Textile Engineering)
Dr. Alex Hobbs (NC Solar Center)
Mr. Tim Jackson (Fluor)
Dr. Prachuab Kwanyuen (NCSU Department of Food Science)
Mr. Brian Ketchem (NC Department of Transportation)
Mr. Rick Lawless (Wyeth)
Mr. Shawn LeMond (Elizabeth City Glass)
Dr. Jim McClain (Micell Technologies)
Dr. David Ollis (NCSU Department of Chemical and Biomolecular Engineering)
Ms. Joan Patterson (NCSU Department of Chemical and Biomolecular Engineering)
Mr. Al Perez (Wyeth)
Dr. George Roberts (NCSU Department of Chemical and Biomolecular Engineering)
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# Two-Minute Project Overviews

**9– 9:45AM, Room 1011**

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**10 – 11:30AM**  
Poster Session (First and Second Floor Atrium of EB1)

**11:30 – Noon**  
Closing Remarks and Special Recognition (Room 1011)
Rising oil prices over the past decade have prompted more in depth investigations as to the feasibility and practicality of the production and use of fuel ethanol. Furthermore, the production and use of ethanol from renewable resources appears to be more environmentally sound than it petroleum-based counterpart. Current trends show that ethanol production and use is increasing rapidly, and could ultimately contend with petroleum-based fuels as a primary source of energy in the United States. The goal of this project was to evaluate the feasibility and practicality of a farm-scale ethanol production facility using transgenic industrial sweet potatoes as a primary feedstock. Through the use of this novel feedstock, it was hoped that the process could be economically feasible and practical, especially to North Carolina farmers. A thorough analysis of the costs associated with implementing this process suggests that it is currently not economically favorable to do so. Substantial governmental subsidies and incentives are available for this type of facility, however they are unable to counter the current overall unfavorable economics.

Briefly, this project sought to improve the economics of this process through several primary modifications including: 1) the use of a novel transgenic feedstock 2) the use of industrial sweet potatoes 3) the use of a more efficient fermentation organism (*Zymomonas mobilis*). The project inherently focused reducing the costs of enzymes used for hydrolysis. The initial thought was that using transgenic sweet potatoes with an intrinsically thermostable hyperthermophilic enzyme would reduce, if not eliminate, enzyme costs associated with the process. This apparently clever modification proved ineffective in reducing the overall cost of producing ethanol. With that in mind, and due to a public reluctance to accept transgenic species, the use of this type of feedstock may not be particularly desirable at this point. A second modification to the process, which focused on reducing the cost of feedstock production, was the use of industrial sweet potatoes. This more resilient feedstock would favor mechanical over traditional manual labor, thereby decreasing harvesting costs by as much as 20%. This proved to be the most economically advantageous modification. The third primary modification was to use a fermentation organism (*Z. mobilis*), which was more efficient than traditional yeast. It was found that the use of *Z. mobilis* would increase ethanol production and reduce fermentation time. Though both of these modifications improved the economics of the process, they were not substantial enough to consider the process economically favorable.
Industrial Production of Beta-Lactam Antibiotics

Nathan Bowers, Adele Hodges, Philip Welch
Advisor: Dr. Steven Peretti

After completing a thorough analysis of all facets of pharmaceutical facility design, including selection and sizing of most unit operations, process simulations, and consideration of relevant environmental and regulatory concerns, BetaCorp suggests that funds be allotted for the construction of a production plant for β-lactam antibiotics with a capacity to produce at least 350 tons of cephalosporin intermediates per year. β-lactams represent a vibrant market that has shown consistent growth while accounting for a large portion, up to 78.3%, of the total global antibiotic market. Cephalosporins were chosen as a product since they have traditionally accounted for a large portion of β-lactam sales, and are effective against a wide range of pathogens. Though it is extremely costly for a start-up facility to pursue the production of a novel, patented, “designer” drug, the production of the semi-synthetic cephalosporin intermediates 7-ADCA, 7-ACA, and 7-ADAC does represent an attractive option. The existence of an established antibiotic market indicates that there will be a stable demand for these intermediates upon which semi-synthetic cephalosporin antibiotics are built.

Therefore, BetaCorp has determined that a viable corporate strategy will involve partnerships with established pharmaceutical corporations in order to form a solid foundation. BetaCorp will provide low cost intermediates in exchange for the supply of proprietary information, such as microorganism strains and substrate compositions. Equity in the company will be offered in exchange for financial assistance in covering start-up costs associated with the construction of a new $390,000,000 facility. Current work has involved the development of a process model based on established recombinant gene expression, fermentation technology, and downstream processing techniques. Fermentation of organisms capable of recombinantly producing acylated cephalosporin compounds in the fermentation broth is followed by primary recovery, involving removal of biomass and other contaminants through filtration or centrifugation. BetaCorp has developed a process that is theoretically capable of improving upon the current industry standard for cephalosporin product yield by 84%, and producing a final cephalosporin intermediate titre that is 99.98% pure.

SuperPro® was used to create a working simulation of the procedure, and to develop specific process alternatives to create an optimum product yield. SuperPro® has predicted that one 200,000 liter fermenter is capable of producing just over 60,000 kg of cephalosporin per year, while generating $240,000 in profits. At this rate, approximately six fermenters of this size will be necessary to achieve the production of 350 tons of antibiotic, thus earning a total of just over $1.5 million. Comparing these figures to the cost that would be incurred in constructing and operating a facility of this nature, this process does indeed represent an economically feasible venture, provided that corporate partnerships are established and outside financiers contribute to initial capital investment.
Biodiesel Synthesis from Waste Oils

Wes Brummer, Brandon Sessoms, and Clint Thrasher
Advisor: Dr. Steven Peretti

The current industrial society is largely dependent on cheap energy sources for continued growth. Currently, petroleum fuels serve as a main source for energy in the United States. However, there is a growing concern surrounding energy security in the United States. As global supplies of petroleum dwindle, new sources of energy must be developed to ensure continued economic growth in the United States.

Biodiesel has come to the forefront as a renewable alternative energy source. Furthermore, the combustion of biodiesel has lower emissions levels than those of petroleum diesel. Another attractive advantage of biodiesel is that it can be produced from many vegetable oils, including waste cooking oils that are generated from fast food restaurants. Waste cooking oils are an ideal raw material for producing biodiesel because it is both abundant and inexpensive.

The current technology for producing biodiesel converts waste cooking oil through a base catalyzed transesterification reaction. The process for this reaction uses waste cooking oil with methanol in the presence of an alkali catalyst (potassium hydroxide) to react the triglycerides to produce alkyl esters as biodiesel. The alkali-catalyzed reaction is sensitive to the free fatty acids and water found in the waste oil, which causes the formation of soap and glycerol as side products. However, with the use of acid catalysts the production of glycerin is reduced and the presence of water is eliminated because the acid catalysts are not sensitive to the free fatty acids that are present in the waste oil.

The project will involve a design of a process that is capable of producing 5000 gallons a week of high-quality biodiesel using the technology of alkali-catalysts and acid-catalysts with waste cooking oil. A cost and profitability assessment will be done for the process capable of producing 5000 gallons a week of biodiesel to quantify the pilot scale process. Investigation of alkali-catalyst and acid-catalyst will be included to determine the optimal catalyst. Also, other investigations of pretreatment of waste oil, separation processes, and mixing will be included to determine if they are feasible and economically valid. Once optimal reaction conditions are determined, there will be a formulation of how the process should work on a larger scale. A comprehensive and thorough economic assessment will be done for pricing of raw materials and equipment needed for the final design. The cost of biodiesel produced from the optimal process will be compared to current and projected diesel prices.
Elizabeth City Glass Recyling

David Day, Alan Johnson, Frank Shaffner, and Robert Williams
Advisors: Mr. Brian Ketchum and Dr. Lisa Bullard

Elizabeth City Glass (ECG), of Pasquotank County North Carolina, processes consumer waste glass to produce a concrete-grade aggregate. ECG utilizes its glass aggregate to produce concrete garden stones, curb stops, and dimple strips. The North Carolina Department of Transportation (NCDOT) is interested in ECG because of the potential substitution of glass aggregate for rock aggregate in structural concrete. The NCDOT is motivated to pursue this because federal and state mandates require that recyclable materials be used in all government operations if feasible. The NCSU Senior Design Team, ChE Glass, is helping ECG by proving to the NCDOT if ECG can consistently produce a viable glass aggregate.

The team developed a laboratory procedure in accordance with ASTM C 40 and performed tests on ECG’s aggregate product, during timed intervals, to determine if it passed as a clean aggregate. Turbidity tests were performed on ECG’s process wash water in hopes of correlating the wash water turbidity to the results of ASTM C 40. As a result, ECG would scientifically have a relationship between aggregate viability and process time. The outcome of these tests would also determine if any costs could be saved in eliminating the need for treating wastewater discharged from the glass cleaning process. An economic analysis was performed to weigh the manufacturing costs of glass versus rock aggregate. In addition to the economic analysis, the team also examined the problems associated with producing concrete mixtures. If the sugars present on the glass entering the process are not fully removed by the wash water, then these sugars can retard the concrete curing process. Therefore, the team calculated the sugar solubility limit and the total organic carbon (TOC) of the wash water to determine if sugar was a concern for concrete mixtures. The Alkali-Silica Reaction (ASR) of concrete was also investigated for ECG. Finally, the team attempted to determine the glass throughput of the process.

All glass exiting the process passed ASTM C 40, except at process start-up, which eliminates the need for wastewater treatment. At process start-up, glass remains in the wash water from batch to batch, and sediments collect on the glass surface. The wash water sample corresponding to this aggregate sample displayed a spike in turbidity above 4000 NTU. It is recommended that the wash water system be run for about fifteen minutes prior to batch start-up to ensure that the glass remaining at the bottom of the wash tank is clean. These tests prove that ECG can consistently produce clean glass aggregate during the time of one batch. An economic analysis proved that it is cheaper to manufacture glass than rock aggregate. Using glass as an aggregate saves money in the future while reducing the amount of glass in landfills. Solubility limit and TOC results of the wash water show that the sugar concentration in the wash water can be neglected; this pertains to a minimal concentration of sugar on the glass. To deter the ASR, it is recommended that ECG introduce calcium ions in the wash water. Unfortunately, the only goal unachieved was the calculation of maximum glass throughput. This was not determined because ECG did not possess necessary documentation. For this reason, the team recommends ECG keep better batch records. Adopting these recommendations will allow ECG to produce a consistently clean aggregate in accordance with NCDOT standards.
Board Number: 5

Citric Acid Production

John Berger, Sarah Geouge, Shelly Heath, Christina Rossi
Advisors: Mr. Tim Jackson, Dr. Steven Peretti

In 2002 citric acid sales were estimated to be $1.2 billion worldwide, making it a very profitable industry. U.S. participation in the worldwide market only accounts for three out of the top ten companies, all of which focus on production of food grade citric acid. Shifting attention to production of industrial grade citric acid for industrial applications, such as metal cleaning and detergents, poses a chance for significant profitability due to the lack of competition in the domestic market. In addition, as the market for detergents is expected to increase by 4.6% and 2.6% for other industrial uses, entry into the US market proves all the more enticing.

This project involved the design of an industrial facility operating 330 days of the year and capable of meeting the specified annual production rate of 20,000 tons of industrial grade citric acid. The analysis focused on a concept design with a detailed process flow diagram (PFD) being the main deliverable. A process description, as well as an economic analysis, accompanies the PFD. All equipment, operating conditions, and locations of intermediate tanks are included. Specific parameters, including titer options, purification method, and number of fermentors, were critical decisions within this project and followed from the mass and energy balance calculations.

In particular, titer option 1 required 140 g/L of citric acid to leave the production fermentor, while titer option 2 resulted in 120 g/L exiting. The number of seed and production fermentors followed from analysis of these two titer options. The two purification methods included precipitation purification and liquid-liquid extraction. Precipitation purification involved the recovery of citric acid as a precipitated calcium salt, while the liquid-liquid extraction method required the separation of citric acid from the crude fermentation broth using a water-immiscible organic extractant.

Based on the simulation data, 3 seed fermentors and 9 production fermentors are required for titer option 1, and 4 seed and 8 production fermentors are needed for titer option 2. Improved scheduling between the seed and production fermentation stage is responsible for the lesser number of required seed fermentors than production fermentors. Between the two purification methods, precipitation purification experienced a 40% loss in product while liquid-liquid extraction saw a 32% loss. Economically, precipitation purification had a Rate of Return on Investment (ROROI) of -4.21% for titer option 1 and -4.66% for titer option 2. Liquid-liquid extraction saw a ROROI of -5.8% for titer option 1 and -6.18% for titer option 2. After extensive review of SuperPro simulation data, it was determined that SuperPro’s focus on pharmaceutical applications was most likely the main cause of the negative ROROI for all options. Based on simulation data alone, the current facility will not prove profitable and should not be constructed; however, more research into SuperPro’s cost analysis will most likely result in a positive ROROI and the design facility should then be implemented.
Kema, Inc., a small lotion manufacturing company in North Carolina, specializes in three lotion products: body lotion, hand cream, and face cream. The company contracted the Lotion Manufacturing Design Team to explore the possibility of reducing manufacturing costs by developing a continuous production process that could replace the current batch process equipment at the end of its operating life. This project goal involved evaluating both the product formulations and the production equipment. This allowed the Design Team to recommend that a process switch would be beneficial to the Kema plant.

The Kema lotion formulations consist of an oil phase and a water phase that are mixed together to form an emulsion. When laboratory testing was done, the body lotion was initially too thick for proper dispensing, so the formulation was adjusted accordingly by changing the water phase to oil phase ratio, which resulted in the desired consistency. The lotion did not leave a greasy feeling on the skin, rubbed in easily, and caused no initial undesired effects on the test subjects when applied properly. The densities of both phases were measured to assist in sizing process equipment.

The team calculated a capacity for the continuous process based on production requirements, assumptions for operating time and down time, and projected market growth. A basic PFD and description of the process were generated to determine the necessary equipment technology and specifications. Subsequently, process equipment was chosen from various vendors and sized appropriately.

Both the existing batch processes and the designed continuous process were simulated in SuperPro Designer®, and the results were used to perform a cost analysis. The two processes were also compared in terms of technical feasibility, flexibility, efficiency, environmental impacts, and quality control. This information was used to assess the viability of a process change at the Kema plant.

In all of the comparison categories listed above except flexibility, the continuous process proved to be the better option. The concern with flexibility is minimal with respect to the benefits of the continuous process in all other areas of evaluation. In addition, an analysis of capital investment and annual operating costs showed that installation of the continuous process would cost approximately 60% less than replacing the current batch process with identical batch equipment. For all of these reasons, the Lotion Manufacturing Design Team recommends that Kema, Inc. implement the newly designed continuous process when the current batch equipment is replaced in their Small Town, NC plant.
Over the past 8 years, the use of poly(ethylene terephthalate) (PET) has increased over 150% in America and continues to grow each year. This increase is due mainly to the use of this high chain polymer in beverage and food packaging. With this large demand, virgin PET will eventually become more expensive and the large amounts of post consumer PET not being recycled will overrun landfills. This project will determine the production capabilities of a proposed depolymerization process for a portion of a large-scale PET recycling facility. Research being conducted by Joan Patterson has shown that recycling PET for food grade packaging can be improved compared to current processing using a new depolymerization process. The process involves the use of a twin-screw extruder, supercritical CO₂ and a glycolysis reaction in a single unit process to depolymerize PET into viable low molecular weight product. Extensive research of available technologies of these three main unit operations guided the design of the scale-up process.

This scaled up process being proposed is a slight purge system which processes ~2000lbs of clean flake PET per hour. The system processes the PET in a twin-screw extruder; supercritical CO₂ to plasticize the polymer. Plasticizing the polymer cleans and expands it to allow the EG to depolymerize the PET. The depolymerization process will create a final product with an N value between 6 and 10 that will eventually be repolymerized into PET for viable use in food grade packaging.

The capital investment for the project including all equipment and installation will cost approximately $2.3 million with a yearly operation cost of $4.6 million. This will include 7 full-time employees, all raw material and energy expenditures as well as an estimate for maintenance of equipment. Cost analysis shows final product should be priced at $0.33, creating net profit after 3 years of operation. This corresponds to an increase of $0.13 per pound of PET processed from start to finish for the depolymerization process alone. The recommendation for this project is the slight purge system based on calculations done and by comparing the cost analysis for each process. Given confirmation of all calculations experimentally, the system will not produce purity needed for repolymerization, but will process high molecular weight PET into a low molecular weight product.
BBEC has requested the design of a grass roots plant to manufacture 120,000 tones of ethylene oxide per year. Ethylene oxide is the major intermediate in numerous applications, including ethylene glycol; ethoxylates; ethanolamines; diethylene, triethylene, and polyethylene glycols; and glycol ethers. Fifty percent of ethylene oxide’s major applications comes from the production of ethylene glycol, and approximately two-thirds of ethylene glycol goes into the manufacturing of polyethylene terephthalate (PET). PET is widely used in the production of fiber, film, bottling, and engineering resins. Current market studies are forecasting healthy growth for the demand of ethylene oxide and its major applications over the next six years. Ethylene oxide is expected to grow at 3.55 percent per year due to the increase in demand of ethylene glycol and PET. The current market for ethylene oxide is 14.75 million tonnes per year and is expected to reach 19.5 tonnes per year, by the year 2010.

Ethylene oxide is produced when ethylene is fed to a reactor with excess oxygen in the form of pure oxygen or purified air. SuperPro Designer software was utilized to simulate four major different process alternatives in the production of ethylene oxide. These alternatives include oxygen fed to an isothermal reactor, oxygen fed to an adiabatic reactor, air fed to an isothermal reactor, and air fed to an adiabatic reactor. Economic reports and stream reports were also generated for each of the process alternatives. An economic analysis along with a ten percent after tax rate of return was conducted. The startup cost and the operating cost of each process alternative were also determined. All of these analyses were used in determining the best process alternative for the design of the facility.

After completing all of the economic analyses and looking at the startup cost and the operating cost of each of the process alternatives it was determined that the project should be carried out and that the oxygen fed to the adiabatic reactor should be used in the design of the facility. The oxygen fed to the adiabatic reactor was superior to the other alternatives in every analysis that was conducted. It had the lowest unit production cost at $0.77/kilogram, compared to $0.80, $0.90, and $0.95/kg for the other alternatives. The oxygen fed to the adiabatic reactor also had the lowest selling price needed to achieve a ten percent after tax rate of return at $0.75/kilogram compared to $0.90, $0.91 and $1.19/kg for the other alternatives. The startup cost was the lowest of the four alternatives at $141,519,000. The operating cost was also the lowest of the four process alternatives -- $76,886,000 per year. The average selling price for ethylene oxide is currently around $1/kg; therefore, designing this facility using oxygen fed to an adiabatic reactor has the potential to be very profitable.
Residential Applications of Hydrogen Fuel Cell Technology

Michael Guthrie, Chad Herr, Whit Rawls, and Kim Sutton
Advisors: Dr. Peter Fedkiw and Dr. Lisa Bullard

This project investigates hydrogen fuel cell technology as a source for residential heat and electrical power. The existing natural gas infrastructure will supply the fuel cell power system with a source for hydrogen fuel. Residential energy demands, including peak, base-load, and geographic factors, will be defined to identify the required energy outputs of a combined heat and power system. Several different types of fuel reforming methods, as well as fuel cell technologies, will be examined in order to choose the optimal residential system design. The complete system will combine these two subsystems with a power conditioning unit and a method for thermal cogeneration. The societal benefits and profitability of incorporating fuel cell power units into the residential sector will be evaluated through an environmental and market analysis by comparing our design to the current distributed power grid.

Current available technology suggests that the ideal residential fuel cell system will utilize an autothermal reformer and a proton exchange membrane fuel cell. Based on residential energy usage profiles and lifetime degradation considerations, the optimal system capacity was found to be 5kW. The fuel cell stack will contain 476 fuel cells which each have surface areas of .0025 cm². The volume of the fuel processing system is estimated to be 5.58 L. To operate the 5kW fuel cell, the autothermal reforming system requires 62.2 mol/hr of natural gas and is capable of producing 166.6 mol H₂/h. The fuel cell unit is also expected to produce 25,587 BTU/hr of thermal energy, a portion of which will be recovered by a cogeneration system and used for residential heating. The cogeneration system will consist of four heat exchangers with heat transfer areas of 0.47, 0.61, 0.42, and 0.62 m², a heat transfer fluid, and a thermal storage tank. It has been estimated that emissions from the fuel cell system will contain 2.72kg CO₂/hr. CO, SOₓ, and NOₓ emissions are negligible and particulate matter releases are eliminated entirely.

The capital cost of the system is expected to be $52,411.20, with an annual cost of $3,585.26. The total lifetime cost of the fuel cell has been found to be $88,263.80.

High volume production would be the most effective means of decreasing the initial cost of the system. The rapidly rising costs of natural gas (current national average of $11.44/1000ft³) could make operating costs a concern in the future. To become more practical, alternative sources of hydrogen, such as biomass and water electrolysis, could be utilized. Also, government tax incentives could be offered annually, as opposed the initial installation credits currently offered. These strategies would help decrease the cost of the system and make it more reasonable for average residential consumers. Overall, the project concludes that the proposed fuel cell power system requires further development before it can be introduced into the commercial market.
Due to the economic and environmental problems involved with the petroleum industry, it is necessary to find other alternative sources of energy. Of the many possibilities for alternative energy sources, biodiesel is one of the most favorable due to its many economic and environmental benefits. Biodiesel is formed through the transesterification of natural, renewable reactants in ethanol, waste vegetable oil, and catalyst; but 10% of this product is a waste stream that is predominately glycerin. Currently local biodiesel producers are composting the glycerin waste, which results in a loss of possible revenue. This affects the biodiesel industry’s ability to keep its cost low since it is losing a portion of material to waste. This loss of possible revenue will only increase with increased biodiesel production. The project proposes to find an economically feasible process of producing a value-added end product from the glycerin waste stream, which may ultimately lower the cost of the biodiesel process.

Two applications for the glycerin stream were determined after examining various markets and specifications. The first application is to purify the glycerin stream to United States Pharmacopeia (USP) grade glycerin to provide the quality and consistency needed to sell to various markets, such as the pharmaceutical, textile and cosmetics industries. The sale of the glycerin would bring in another source of revenue and lower the cost of the biodiesel process. To reach USP grade glycerin, three possible purification pathways were selected to research. The first two (activated carbon and vacuum distillation) were eliminated from consideration due to the high costs involved with them. The third pathway involves using acid-base separation, batch distillation, and ion exchange chromatography in sequential order and was chosen because it was the most economically feasible process compared to the other two pathways. The second application involves using microorganisms in a reaction with the glycerin to form ethanol, which will either be recycled back into the biodiesel process or sold. Recycling the ethanol would eliminate some of the raw material cost while selling the ethanol would bring in another source of revenue. Both scenarios would lower the cost of the biodiesel process. Two microorganisms (Zymomonas mobilis and Saccharomyces cerevisiae) were selected to test in these experiments because of their optimal growth conditions, propensity to produce ethanol, and other advantages.

Three separate runs were completed for acid-base separation. The first seemed to be successful when it settled out into three phases, but the last two runs gave erratic results. GC/MS analysis of the first run showed that glycerin was present with several other components, though compositions were unable to be determined due to problems with the column. After modeling the two applications with SuperPro™ utilizing mostly information obtained from research, it was found that both of the processes would not recover enough cost to compensate for the operating costs of the facility and were thus not economically feasible. Studies of the purification and reaction processes should halt until ways to circumvent some of the large costs involved.
Development of a Miniature UV-NIR Spectroscopy Apparatus to Detect Chemical Warfare Agents on a Real Time Basis

Mark Mathews, Shane Miller, Joe Rittiner
Advisors: Dr. Juan Hinestroza and Dr. Lisa Bullard

Chemical weapons represent a severe threat to the health and safety of the free world, especially in this age of terrorism. Testing of protective equipment to combat chemical weapons is currently done by the Man-In-Simulant-Test (MIST). In this test, a man wears a protective suit and is placed in a chamber filled with a chemical agent stimulant, a biologically inactive chemical with similar physical properties to the chemical agent. It is then measured how much simulant penetrated the suit, and thus, the suit’s effectiveness can be determined. Currently, the amount of simulant is measured by absorbent pads, which can only measure the cumulative amount of simulant that passes through the suit. Therefore, real time data collection is not possible. In addition, the pads only absorb one chemical, methyl salicylate (MeS), so equipment testing with multicomponent mixtures is also not possible.

A real-time detector system will be developed for use in testing of protective equipment. Ultraviolet-Near Infrared (UV-NIR) spectroscopy will be used to identify the concentrations of simulants inside the protective equipment from the order of parts per million. The use of spectroscopy allows the simultaneous concentration measurement of multiple components. Fiber optic cables will be used to carry the spectroscopic data streams. This allows the sample chamber to be placed inside the harsh testing environment, while leaving the sensitive spectroscopy equipment in a more accommodating location. Computer software will be used to calculate concentration figures from absorption readings, and to collect data. This detector will allow the collection of more complete and accurate concentration data, providing a better foundation for the design of protective equipment.
Cholera Microbusters, Inc. has developed a credit-card-sized microfluidic device for the detection of *Vibrio cholerae*, the bacterium that causes cholera, in drinking water. The device is intended to provide an inexpensive and reliable means for tourists and local health officials in the developing world to determine if their water supply is contaminated with deadly cholera bacteria. The device design relies on the accuracy of an immunometric assay to detect *V. cholerae* cells. Antibodies specific to *V. cholerae* will be immobilized on the detection surface of the device. When a collected sample is passed over these antibodies, any *V. cholerae* cells present in the sample will be captured. Afterwards, antibodies labeled with gold particles will be passed over the detection surface and will bind to these captured cells. Because of the gold colloids, a contaminated sample would result in a reddish color on the detection surface. However, the design also utilizes the recently developed technique of silver enhancement of the gold colloids, resulting in a strongly amplified and more definitive signal. None of the reagents required for these processes has been found to pose an environmental or safety hazard.

Finger-actuated micropumps consisting of elastic silicone-rubber chambers are used to collect the sample and dispense reagents to the detection chamber. Theoretical and experimental analyses of finger-actuated pumps were performed to determine the pump dimensions that would minimize the unused, or “dead,” pump volumes. From these analyses, it was concluded that percent dead volume decreases with increasing pump diameter for the reagent dispensers, increases with increasing pump diameter for the sample collector, and is independent of height for both chamber types. Furthermore, for a set chamber height, a reagent dispenser with a little more than half of the diameter of a sample collector yielded the same effective volume. Because each reagent volume dispensed should fully replace the fluid present in the detection chamber before its release, it was assumed that equivalent effective volumes of reagent and sample are desired. Ultimately, to maximize the effective volume, a height of 0.0625 inches, a reagent-dispenser diameter of 0.625 inches, and a sample-collector diameter of 1.0 inch were selected. The micropumps and channels were arranged on the device so as to maximize convenience for the user. The sample collector and detection chamber are situated in opposite corners of the device to facilitate sample aspiration, and the reagent dispensers are arranged in the order in which they are to be pressed to minimize confusion during operation. A prototype demonstrating the effectiveness of this arrangement, including the optimized micropumps and channel width, has been created and is available for inspection. Three-dimensional schematics have also been generated and are included in the final report.

This final report presents a design in which most of the technical aspects have been analyzed. With a total estimated materials cost of $2.16 per device, this device has major potential to forge a new market of inexpensive, point-of-care diagnostic tools of which tourists, residents, and local health officials can take advantage. To complete development of this design, experimentation must be performed to research the specific effects of device operation on *V. cholerae* cells and to study the appropriateness of the recommended manufacturing techniques.
The pharmaceutical industry must continuously address current industrial and federal regulations that dictate both product approval and long-term product profitability. Drug regulatory administrations attempt to analyze the effects of pharmaceutical products prior to release in order to protect public safety and avoid drug recalls, as was the case with the Vioxx recall. Product protection agencies also prevent the monopolization of pharmaceuticals by limiting the life of pharmaceutical patents. This limited protection allows the production of generic alternatives after a given number of years, which in turn reduces the long-term profitability of the drug. In order to receive initial product approval or extend patent life, drugs must often be re-engineered. This could involve reducing side effects, increasing efficacy or improving the method of production.

This design project attempts to accomplish all three of these improvements for a given pharmaceutical by employing supercritical-based process strategies.

The pharmaceutical product selected for re-engineering is a respiratory medication called albuterol. About 90% of albuterol products used in the U.S. are generic brands, and all albuterol products are racemic. Although many drugs are produced as a racemic product, often only one enantiomer is the active ingredient. Recent studies have shown that inactive enantiomers may actually reduce the effects of the active enantiomers and may be the cause of drug side effects. Although enantiomeric separation technology is limited, many pharmaceuticals, including albuterol, may be improved by separating the two enantiomers. Additionally, the efficacy of respiratory drugs is often a function of particle size, which may or may not be controlled in their production. As a result, albuterol may also be improved by controlling both particle size and distribution. The team developed a process that can separate the two enantiomers of albuterol, and then process the active enantiomer to form a fine powder to be sold in bulk. In order to avoid the use of large amounts of environmentally harmful organic solvents, both the separation and particle formation processes use subcritical and supercritical CO₂ as the main solvent. The separation will be performed by using supercritical fluid chromatography with a chiral stationary phase. The fine particles will be generated using a solution enhanced by dispersion in supercritical fluid which can produce uniform fine particles from 2-5 µm. This design process integrated these two processes to make an industrial-scale process that can produce enough (R)-albuterol to satisfy one-fourth of the current U.S. market demand.

The initial investment for this process came to be about $1 million dollars, which includes capital costs and the initial cost of raw materials. The economical analysis estimated that the initial investment will be paid off by the third year of operation, and profits will start to accumulate thereafter. The net present value is estimated to be $2.3 million. Based on this favorable economic analysis, this report recommends the implementation of this process as an addendum to an existing facility.
A Novel Design and Manufacturing Process for Dye-Sensitized Solar Cells

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This report addresses the feasibility and profitability of producing dye-sensitized solar cells (DSC’s) commercially. First, an analysis of different types of organic solar cells was performed. This analysis allowed for the selection of the most feasible cell to produce. Three device types were chosen for in depth research: dye-sensitized, fullerene, and hybrid nanorod cells. These cells were chosen based on the amount of current research being conducted and also based on the fact that they represent significantly different areas of organic photovoltaic cell technology. Based on selection criteria, including cell power conversion efficiency, availability of materials, and the existence of a manufacturing process, dye-sensitized photovoltaic cells were found to be the most viable choice for this design project.

Upon selecting dye-sensitized cells, an in-depth analysis of current construction processes was conducted. The current construction processes were all based on the production of flat plane rooftop systems. Initially, the aim of the JEK Parson’s Project was to produce DSC’s for rooftop integration. However, since several companies are currently selling flat plane DSC rooftop systems, the project changed direction to focus on and create a more innovative solar cell design. It was determined that there exists an un-tapped market in the area of portable energy production for portable electronics. In order to produce a portable DSC for small electronics, several key issues had to be addressed. The most crucial issue was that of cell size. The energy requirements of a given electronic device directly determine the size of the DSC needed. Being that the device should be easily portable and not cumbersome, mathematical models were developed to optimize the photo-generated current and, consequently, minimize the size of the device. Through quantum mechanical modeling, the optimal photoactive film thickness was determined to be 32.09 µm. An analysis based on the power requirements of handheld GPS devices and the average energy provided by the sun led to a minimum device size of 240 cm². Therefore, a size of 300 cm² was chosen, so as to be larger than the minimum size and still easily portable. Incorporating a diffusion model with the quantum mechanical model allowed for production process optimization, through the determination of the diffusion time that leads to the optimum amount of dye in the cell.

Finally, the cost and profitability of the solar cell production plant were addressed. The market for handheld GPS devices was deemed to be a good representation of that of portable solar cells due to the fact that some type of portable energy must power all handheld GPS units. Even if market penetration is as low as 1%, the market size for portable DSC’s is $350 million. Easily attainable costs of manufacturing, such as machinery, utilities, location, etc. were collected. The cost of materials for a single device was determined to be $62. Based on production capabilities, the maximum number of devices produced is 22 per day. This yields 1.5 million dollars per year in sales, with an individual device cost of $200.
Facility Design: Bulk Pharmaceutical Manufacturing and Packaging

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Biogen-Idec has commissioned a project to design a 3000-liter scale biopharmaceutical manufacturing facility to accommodate a diverse product pipeline of protein-based treatments. Biopharmaceuticals is currently a $35 billion industry with a projected annual growth of 15%. Facilities in this lucrative industry often have a return on investment of 30-40%. With projections for the arrival of 50-60 new biopharmaceuticals into the market by 2009 and for a shortage of production capacity for biopharmaceutical products by 2006, the future of the industry is promising. As a rapidly growing industry, a biopharmaceutical facility has great promise for high economic returns. The design of such a facility calls for expertise in the two broad areas of cell culture and downstream product purification. This requires the development of a process flow diagram along with detailed piping and instrument diagrams for each unit operation. In order for the process to take shape, construction and validation schedules must be developed. This will be justified by an economic analysis of the design, placement, and operation of the facility.

The process under design produces Avonex, a multiple sclerosis drug manufactured by Biogen-Idec that generated $1.1 billion in revenue in 2003. Avonex is a protein-based treatment harvested using a Chinese Hamster Ovary (CHO) cell line. The facility will also be capable of manufacturing a diverse product pipeline of similar protein therapeutics. As typically used in the biopharmaceutical industry the production fermenter operates as a fed-batch reactor at a scale of 3000L. After cell culture is complete, harvesting begins and the protein product is isolated from the cell slurry and purified. Packaging and distribution of the purified product will be contracted out for financial considerations. A detailed process flow diagram (PFD) and accompanying piping and instrument diagrams (P&IDs) are complete. The cell culture process includes stirred-tank bioreactors sized using a mathematical model, which determined that nine stages are required for the scale-up process with a residence time of 45.7 hours per stage. The final purification scheme includes a centrifuge, three chromatography columns (affinity, ion exchange, and gel permeation), two ultrafiltration skids, and one viral filtration skid. The downstream process equipment is arranged based on general purification heuristics and the specific needs of protein purification in CHO expression systems. A basic facility layout that accommodates the process and utility equipment is also complete. Four main objectives drove the design of the facility: facilitate process flow, minimize required clean space, minimize required transport distances, and allocate space for process additions. Generic P&IDs are complete for each process unit and include information on equipment design, control scheme, piping size and material, and equipment IDs.

The total fixed capital costs were calculated to be $151 million for the facility. Annual operational costs are estimated to be approximately $159 million. The facility will be able to generate $2 billion in revenue per year. Annual profits can be estimated at $1 billion per year after taxes and operating costs but before research and advertising expenditures.
ACME Biotechnology, Inc. supplies vaccine manufacturers with a binding protein (BP-1), which is used to produce polysaccharide-protein conjugate vaccines for infants. The company requested that Injectibles, Inc. develop a facility plan for increasing the production of BP-1 based on three alternatives: (1) replacing the current 1500L production fermenter with a 3000L vessel; (2) adding a second 1500L fermenter to the current unit in the fermentation suite; and (3) adding an entire second fermentation train to the existing facility. During the progress of the project, a fourth option was developed based on the design of Option 2, but involved the addition of a 3000L production fermenter. Thus, this option will be referred to as Option 2B. In order to determine the best expansion option, SuperPro simulations were performed in addition to an economic and regulatory analysis. The economic analysis evaluated the costs associated with each option, including raw material, labor, and equipment costs, the BP1 inventory levels from 2005-2010, and the profit obtained over the next five years. The regulatory analysis evaluated the effect of federal laws and standards on the execution of each process option, particularly the effect of validation. ACME Biotechnology, Inc. noted that they could sell as much BP-1 as produced. Therefore, the performed analyses and proposed method of action did not reflect market limitations.

Following the aforementioned evaluations, all options resulted in an increase in cumulative profit and BP1 production from 2005-2010 as compared to the current process, with Option 3 generating the greatest increase of all. However, Option 1 proved to be inefficient because the validation process required 6 months of shut down, resulting in loss of revenue. Option 2A was the least cost effective, despite the addition of a second fermenter, generating the least increase in profit. Option 2B was more cost effective than Option 2A since the cost of adding a larger fermenter was minimal compared to the gain in cumulative profit - Option 2A resulted in an increase of 39% while Option 2B resulted in an increase of 69%. Option 2B was also more efficient than Option 1, resulting in 14% more profit and 16% more BP1 production. Despite the economic benefits of implementing Option 3, this option was the least practical because it required timely and expensive construction. Moreover, the new process modification, the second train, would not be implemented until 2007 due to validation requirements.

Since ACME Biotechnology, Inc. desires a process modification that is both cost effective and time efficient with regards to implementation, Option 2B is the recommended expansion option. The BP1 produced per batch increases from 0.4881kg with the current process to 1.4651kg, while the cumulative production from 2005-2010 increases by 65%. The cumulative profit over the next five years is $62.1 million, which is a 69% increase from the current process. Additionally, the process modification is implemented after 6 months of commissioning, IQs, and OQs. During this period, BP1 production is not interrupted because the production capacity of the current process is utilized. Therefore, Injectibles, Inc. recommends this option because it is cost effective and easiest to implement and achieves the project objectives identified by ACME Biotechnology, Inc. – an increase in BP1 production and profit.
Green Biodiesel Production

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With rising petroleum costs leading to higher prices at the gas pump for the consumer, ways to reduce fossil fuel dependence are being sought by researchers worldwide. In conjunction with the Department of Chemical and Biomolecular Engineering, the Department of Mechanical Engineering, and the Applied Energy Research Lab at North Carolina State University, Hippie Diesel, Inc. was founded to research a green production process for biodiesel.

When Hippie Diesel Inc. was founded in September of 2004, the initial project specifications simply called for a process design for the green manufacture of biodiesel using waste oils and bioethanol. To focus the scope of the project, the group decided to create a process capable of producing approximately 1000 gallons of biodiesel per week. This process would likely be operated in an agricultural setting, and ideally, the operator would not need technical knowledge to operate it. Additionally, the process would be free of dependence on fossil fuels, either in feedstocks or in energy inputs to the process.

Primarily, the group researched a vast array of both technical and unconventional literature to determine the proper path towards design. Various laboratory experiments were subsequently performed, permitting the group to determine the optimum reaction conditions for the transesterification and esterification reactions necessary for biodiesel production, as well as a cost effective method for product separation. Additionally, throughput expectations and preliminary economic feasibility were determined using SuperPro Designer®.

Finally, since the group has determined that the process is profitable, it is recommended that design and construction of this biodiesel facility should proceed pending further investigation. Further experimentation is necessary concerning the esterification and product separation steps of the process. A specialized piping and instrumentation diagram and ultimately, a scaled-down pilot plant should be fabricated before plans are submitted to an engineering/construction firm to begin work on this facility.
Carbohydrate Replacement Using a Soy Protein Derivative

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A collaborative effort between the North Carolina Soybean Grower’s Association and North Carolina State University has been initiated for the purpose of determining the feasibility and economic benefits of introducing a new value-added product to the North Carolina soybean market. The product will be a modified soy protein isolate, MSPI, used as a functional pre-gelatinized starch replacement in food processing applications. The introduction of this product to the market will be based on product value analysis, cost assessments and process design optimization.

The analysis of the MSPI produced in the laboratory consisted of testing both the viscosity as a function of shear rate and the water holding capacity. A pre-gelatinized starch and an unmodified soy protein isolate were also tested identically for comparison. The pre-gelatinized starch was used for functional comparison while the unmodified soy protein isolate was used to determine the effectiveness of the modification. Both the unmodified and modified soy protein isolate were tested at a ten weight percent concentration. The pre-gelatinized starch was analogously tested at a three weight percent concentration based upon findings by Hudson and Daubert in the testing of a modified whey protein isolate. The data revealed the water holding capacity of the modified soy protein was greater than the pre-gelatinized starch and the viscosity data revealed the MSPI to be thicker than the starch and the unmodified SPI. In addition to product analysis, a scale-up process design was completed. Due to the current uncertainty of an exact market demand for the MSPI, a baseline of 100kg/batch was used for design purposes. The type of equipment required has been established, and a list of potential equipment suppliers was identified. In order to appropriately scale the final process design, the initial purchasing cost of the process inputs as well as the market value of the MSPI product must be determined. For the scope of this project the input to the MSPI process is soy meal. More extensive analysis may lead to a recommendation of beginning the process at the stage of whole soybeans. The purchasing price of soy meal is $194.20-$204.20 per ton. The expected sales value of the MSPI will be calculated based upon the an extrapolation from current market value of unmodified soy protein isolate comparable to the value increase from a hot gelling starch to a pre-gelatinized starch. The exact profitability associated with the soy protein isolate modification will be based upon the purchasing cost of the equipment and solvents required for production.

The completion of this project will depend upon a complete analysis of the scaled-up process design. This will provide a basis for the economic analysis, including the required labor, initial capital, and operational costs. Upon establishing an estimate for the costs associated with the pilot scale process, the previously established market value will be used for a comparison to determine the potential economic benefit of producing the MSPI. From this a recommendation for development of this process will be made for the benefit of the North Carolina Soybean Grower’s Association.