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 problems, ranging from the removal of perchlorate from drinking water to the design of a plant to make gelatin as a raw material for local pharmaceutical manufacturers. This year’s teams have designed products including a portable fuel cell and a microfluidic cooling device for microprocessors. 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 22 teams consisting of 104 students from four different academic departments and two colleges could not have been accomplished without your help!

Mr. Jeff Brown (Wyeth)
Dr. Chris Daubert (NCSU Department of Food Science)
Dr. Keith Dawes (NCSU Department of Material Science and Engineering)
Dr. Joel Ducoste (NCSU Department of Civil Engineering)
Dr. Peter Fedkiw (NCSU Department of Chemical Engineering)
Dr. Ron Hill (Encelle, Inc.)
Dr. Alex Hobbs (NC Solar Center)
Dr. Nick Hutson (Environmental Protection Agency, RTP)
Dr. Jeanne Koger (NCSU Department of Animal Science)
Dr. Francis Lambert (Encelle, Inc.)
Mr. Rick Lawless (Wyeth)
Dr. Jim McClain (Micell Technologies)
Mr. Robert McGhee (Kennametal)
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AlphaVax, a vaccine research company in Research Triangle Park, is expanding its operations to include manufacturing vaccines and needs a facility that is fit for production. They will be leasing a facility once owned by Apex Biosciences but need to retrofit this area. The major constraints placed on the design of the facility are the size and irregular shape of the existing facility, the steps of the vaccine production process, and the federal and international regulations governing this process and facility. Using knowledge of these constraints, the AlphaVax team designed an ergonomic overall layout, individual room layouts, and pressure gradients for this facility.

The overall layout features several required rooms: a tissue culture lab, two production suites, a filling suite, a vial wash area, a locker room, and storage areas. These rooms have different regulatory requirements based on the level of exposure to biohazardous materials. To enter the manufacturing area, for example, employees must gown into scrubs in a locker room. The vaccine production suites are governed by more stringent regulations that require additional gowning in separate gown-in and gown-out rooms. Similarly regulated areas are grouped within the facility due to gowning requirements and also in order to simplify air handling.

Additionally, certain spaces have features dictated by the process steps. In the highly regulated areas, product will exit through the gown-in rooms while waste exits through the gown-out rooms. As a result, the product flow is kept separate from the waste flow, and the risk of contamination is minimized. The filling suite will be adjacent to the vial wash area to allow vials and other glassware to pass from the vial wash, through an autoclave, directly into the filling suite, eliminating the need to carry sterilized vials through an unregulated area. Furthermore, equipment was placed in each room based on the size of each piece and the relative order of use set by the vaccine production process.

Pressure gradients are used to generate airflows that confine harmful particles and prevent contamination of the vaccine solution. The manufacturing area will be kept above atmospheric pressure, causing air to flow out and minimizing contamination by particles from outside of the facility. To contain viral particles in the production suites, the gowning areas at the entrance and exit of each suite are “supercharged” with even higher air pressures, preventing air from escaping the production suites and also preventing air from the rest of the building from entering the production areas. This system ensures the safety of employees and the vaccine recipients.

If the anticipated HIV vaccine is successful, AlphaVax will most likely gain additional contracts for more profitable vaccines, such as malaria or cancer vaccines, resulting in an estimated rate of return on investment of 8% or more by the year 2025. The AlphaVax team recommends this project because it shows potential for being profitable, meets all necessary requirements, and allows for the manufacture of vaccines that will benefit humanity.
Overall goals for the ammonia plant retrofit can be broken into three major components. These components include: comparing the cost of ammonia production using either a single pressure or a dual pressure process, determining the environmental and economical feasibility of the preferred process, and addressing health and environmental issues involving liquid ammonia. This project evaluates the production of 3000 metric tons per day of liquid ammonia. The equipment and the other necessary specifications have been determined in order to evaluate economic and environmental feasibility.

Because the thermodynamic data given in the project description was not compatible with SuperPro®, the reactor information for both processes has been simulated in Aspen. There was only one exothermic, equilibrium-limited reaction considered in the simulations:

\[
N_2 + 3H_2 \leftrightarrow 2NH_3
\]

The single pressure process utilized only one reactor whereas the dual pressure process had two. Moreover, the dual pressure process had an additional compressor, condenser, and hydrogen selective membrane.

The reactor information has been inserted into the SuperPro® simulation in order to complete stream and energy tables. Using the simulation as well as information found in Turton, et. al, all equipment costs have been calculated and used to determine the bare module cost. The bare module cost for the single pressure process was found to be $84,544,000 and was $72,478,000 for the dual pressure process. The most costly pieces of equipment were the compressors. This information, along with utility, waste, and operating costs provided by SuperPro®, has been used to determine the annual operating cost and the minimum price of ammonia in order to achieve a 10% rate of return on investment. For the single pressure process, the annual operating cost was determined to be $181,123,000, and the minimum price of ammonia in order to achieve a 10% rate of return on investment must be $262/MT. Additionally, if the ammonia produced could be sold at the current market price of $315/MT, the rate of return on investment would be 23.4%. For the dual pressure process, the annual operating cost was established to be $189,934,000, and ammonia must be at a price of $239/MT in order to obtain a 10% rate of return on investment. At the current market price, the rate of return on investment would be 25.2%.

In conclusion, the recommendation of this project group is to build the dual pressure process instead of the single pressure process. Both processes produce 3040 metric tons per day of liquid ammonia thereby producing equivalent emissions. There is an increase in annual operating cost for the dual pressure process of 4.8%. However, the total initial investment for the dual pressure process is 13.4% less than for the single pressure process. Finally, the overall rate of return on investment is 1.8% higher for the dual pressure process.
Biodiesel Facility Utilizing Waste Vegetable Oil

Ryan Adams, Paul Box, Cameron Cobb, Mara Ondeck, Bryce Sturtevant, Stephen Walser
Advisors: Dr. Steven Peretti and Dr. Alex Hobbs

Given the growing uncertainty surrounding energy security in the U.S. coupled with the desire for more environmentally friendly fuel, research into alternative fuel sources has become increasingly important. The production of renewable fuels has the potential to increase national security, reduce harmful emissions, and stimulate the economy. Much research and development is ongoing for the use of renewable fuels referred to as biofuels. Of these biofuels, biodiesel is one that shows great promise as being a sustainable alternative to petroleum-based diesel fuel. Although biodiesel is a renewable, cleaner-burning alternative to petroleum diesel, it is currently more costly to produce. The majority of biodiesel is produced from virgin oil feedstocks such as soybean oil. Since virgin oils are costly, less expensive alternative feedstocks are needed. This project focuses on the design and economic analysis of a community-based biodiesel production facility in North Carolina. This medium-sized plant will process 5,000 gallons of waste vegetable oil (yellow grease) per week into biodiesel primarily for off-road use farm use.

A batch process utilizing a two-step sequence of catalytic reactions will be used to produce the fuel. The first step reduces the amount of free fatty acids (FFAs) in the yellow grease using an esterification reaction over an acid catalyst. The second step of the process is a base-catalyzed transesterification reaction of triglycerides. The primary product, biodiesel, and secondary product, glycerin, are then separated and purified. The FFAs in yellow grease can be effectively reduced to nearly 1 wt. %, which is a requirement for eliminating the effects of soap formation in the transesterification reaction. Therefore, adding a pretreatment esterification step allows for better transesterification reaction conversion. This transesterification reaction proceeds to equilibrium quickly, minimizing reaction time necessary for conversion of triglycerides to crude biodiesel. This crude biodiesel requires purification, and a feasible purification method is achieved through one dilute phosphoric acid wash followed by two water washes. To characterize the fuel properties of the purified biodiesel, samples were sent to the North Carolina State Motor Fuels Lab. The kinematic viscosity and flash point of the fuel were tested and results were comparable with the ASTM standard. The experiments allowed the PFD to be finalized; however, for the facility to be physically realized, an economic analysis was necessary. The cost of manufacturing biodiesel is $1.26 per gallon, which is significantly lower than the commercial price of diesel. The profitability of the facility was evaluated with time, cash, and interest criteria. These factors endorse the construction of the facility given the payback period of 1.15 years, net present value of $329,670, and an internal rate of return of 56%

Although this process is economically and physically feasible, some improvements are recommended for consideration. If production rates were increased, heat may be needed to expedite the two reaction rates. Since a continuous process is necessary at high production rates, further investigation into kinetics and reactor design is suggested. Whether at high or low production rates, biodiesel can be used to generate the facility’s power for a further decrease in production costs.
Ethanol and methanol have been widely considered over the past several years as alternative fuels to gasoline due to the fact that world oil reserves are estimated to be gone within the next forty years. Environmental analyses indicate that there are several advantages to these fuels, including the fact that they have reduced emissions and give higher performance as compared to gasoline, and very inexpensive modifications need to be made to cars so that they can be run on these fuels.

It has been proposed that ethanol and methanol can be produced via biomass fermentation. Using corn and corn stover as substrates, enzymes will be added to cleave $\alpha$-1,4-glycosidic bonds and reduce these complex carbohydrates to glucose, which will then be fed to yeast and bacteria, respectively, to produce ethanol and methane in a batch fermentation. The methane will then be gasified to methanol through a catalytic reaction. Both products can then be purified for distribution.

A major simplifying assumption was made with regard to the methanol process: a bench-scale experiment could be scaled up to 60,000 liters. Block flow diagrams for both these processes were generated, and SuperPro® simulations were then developed to simulate each design. A 12% conversion of biomass to ethanol was generated, however, only a 1% conversion of biomass to methanol was achieved.

Based on these conversions, total cost and market analyses were performed to determine profitability of these products as fuels. The market analysis showed that there was a comparable market of ethanol with gasoline; however, there was a much smaller market for methanol, indicating that ethanol would be a better alternative fuel choice in terms of profitability. Cost analysis proved that the rate of return of investment for the ethanol and methanol designs were -11.3% and -11.2%, respectively.

Even though the environmental and market analyses indicated that these two fuels are safer than and can be just as profitable as gasoline, the cost analysis determined that no further steps should be taken in attempting to produce these alcohols via the simulations proposed by this project. Instead, it is recommended that additional product lines be investigated for optimization purposes. Future research should also be performed to determine a more optimal route of fermentation for both of these processes, since the conversions of biomass to ethanol and methane were low.
Ceramic Processing

Spalding Craft, Laura Creech, Jennifer Schaefer, Diep Vo
Advisors: Dr. Keith Dawes, Dr. Lisa Bullard

The sponsoring company manufactures a ceramic component made of ceramic tape. Multiple layers of ceramic tape are laminated together and fired to produce a component containing an internal cavity. Since the production of the component began in 2000, yields have varied between 5% and 70% due to cracks forming around the internal cavity. This company has asked North Carolina State University to recommend process alternatives to decrease the number of defective parts and improve yield. This report presents an analysis of three process alternative concepts and provides recommendations for future work, based on the team’s experimental investigations.

The major objectives and accomplishments for the team include the construction of an analogous component for basis comparison and investigations of process alternatives. The team constructed an analogous component following the company’s current processing parameters and compared the crack lengths in the analogous part with crack lengths in parts made using the following process alternatives: alteration of lamination pressures, alteration of lamination sequence, and the use of a plasticizer. An increase in crack lengths was seen when the lamination sequence was altered. Decreases in crack lengths were seen with alteration of lamination pressures and the use of a plasticizer. An additional experiment was performed using a half-sample to investigate the surface of the cavity layer. Profilometry data showed curvature on the surface that may decrease contact between the cavity layer and the layer above the cavity.

Based on the experimental results, the team recommends areas for further investigation. Constructing and analyzing more half-samples could pinpoint the step in the manufacturing process when surface curvature of the cavity layer begins. Specifically, the use of a bisque fire on a half-sample could determine whether or not curvature is present before the sintering step. The results of the experiments altering the lamination pressures and using a plasticizer demonstrated decreased crack length. Therefore, the team recommends further investigation of combining altered lamination pressures with the use of a plasticizer. Improvement of the plasticizer application method should be made to control the amount of plasticizer applied to the component.
Citric Acid Production Facility Case Study

Catherine Anderson, Chan Lee, Jimmy Pfeiffer
Advisor: Patty Niehues

This report examines the options available to an existing citric acid facility that has been appropriated funds for modification or expansion. The current facility annually produces 50,000 tons of USP grade citric acid. Management would like to either perform a retrofit and produce a different product or expand to produce more citric acid or a different product. The current facility produces citric acid via a submerged fermentation process, using the fungi Aspergillus niger, so the team chose lactic acid as the alternative product to investigate based on its similar production method and potential market growth. Using SuperPro® Designer 5.0®, the design team simulated all three options and performed an economic analysis to determine which option is most profitable and make a final recommendation accordingly.

Based on past analysis of citric acid and lactic acid production, a hypothetical process flow diagram representing one production line for each product was designed using SuperPro. One production line can produce either 20.1 tons/batch of citric acid or 23.5 tons/batch of lactic acid. Based on an expansion of an additional 20,000 tons per year, the existing plant would need 14 more production lines for citric acid and 12 extra production lines for lactic acid, with both processes running 71 batches per year. A schematic of each design is presented, along with explanations of all process units and any simplifying assumptions the team made.

Based on the process designs developed and the current selling price of citric and lactic acid, $0.55/lb and $0.72/lb, respectively, the expansion efforts resulted in negative rates of return on investment (ROROI). Specifically, the citric acid expansion had an ROROI of -16.6% and the lactic acid expansion of -13.8%. The retrofit also gave a negative rate of return. These negative returns were largely due to two reasons: high operating costs and low revenues. The group tried several ways to optimize the process by reducing some of the high operating costs and increasing the amount of product per batch. The specific scenarios investigated to minimize costs were a reduction in the number of pieces of equipment, a reduction in batch times, and a dual reactor scenario in place of the single production fermenter. Each attempt at optimization created even lower returns on investment.

Based on this evaluation of the proposed modification and expansion options, the team recommends that none of the three options be pursued. We recommend the appropriated funds be used to streamline the current facility to make it more economical and efficient. The team believes the best chance for a solid profit would be to invest back into the original plant.
Production of an Antigenic Co-Protein Line for PeptiVax Pharmaceuticals

Ashley Amstutz, Paige Auten, Eston Herring, and Michael Swanson
Advisor: Patty Niehues

Currently, six million Americans are living with Hepatitis B Virus (HBV), Hepatitis C Virus (HCV), Human Immunodeficiency Virus (HIV), or Respiratory Syncytial Virus (RSV). PeptiVax Pharmaceuticals is proposing four distinct co-proteins as a form of treatment for each disease. Historically, the first vaccines were made using a dead or weakened diseased cell. This dead or weakened cell was then introduced into the body, stimulating the production of antibodies. Since then, other vaccines have been made using the surface poly-saccharide of the disease cell and not the cell itself. This method produces the same immune response without the risk of contracting the disease. However, immune systems of children under the age of 2 years do not have the ability to recognize the poly-saccharide and acquire no immunity from the vaccine. Therefore, PeptiVax has created a treatment using conjugated proteins by removing the antibody response producing poly-saccharides from the outside of disease cells, and attaching the poly-saccharides to a harmless host protein. This polysaccharide-protein combination is capable of stimulating antibody responses in both young and mature immune systems. This project is limited to the production of the host protein, an intermediate for the final co-protein treatment.

Research conducted on current market size and similar drug treatment schemes for each disease led to the calculation of specific production rates and requirements. Comprehensive Super Pro Designer simulations of each co-protein were created based on stoichiometric and kinetic modeling of fermentation with an Escherichia coli host. In addition, associated costs have been established through an evaluation of production requirements, accurate equipment sizing, and waste treatment for a preliminary cost of manufacturing. Based on a ten percent rate of return on investment, ROROI, a selling price for each co-protein was determined.

The cost of raw materials initially constituted the majority of the total cost of manufacturing; this area was further investigated for cost optimization. A price adjustment on the buffer solution, one of the most expensive of the raw materials, was researched and implemented. After the introduction of this new buffer price, the rates of return on investment for each co-protein were recalculated. Co-HBV and co-HIV were shown to exhibit an ROROI lower than the desired value, while co-HCV and co-RSV demonstrated rates of return much greater than the desired ten percent. However, the cost of manufacturing was simplified by not including validation and piping costs, and therefore will need further modification. Also, the ROROI was calculated based off of the consumer price, which consequently includes insurance and other intermediate costs not applicable to the ROROI calculation for this project.

Based on the initial feasibility analysis conducted using the base-line Super Pro simulation, it is recommended that PeptiVax move forward in the production of co-HCV and co-RSV. Further research and data on validation and piping costs, insurance costs, and possible manufacturing modifications will be required to form a final recommendation regarding the economic feasibility of the co-HBV and co-HIV processes.
Innovative Design of a Snowboard

James Carnell, Jackie Gerken, Matt Kain,
Natalie Killmon, Lauren Killough, Courtney Pate, Will Salley
Advisors: Dr. Rich Spontak, Dr. Joel Pawlak

The need for continued development within the most energy-intensive industries in the US has been acknowledged for some time. The Department of Energy’s (DOE) Energy Policy Act of 1992 required these industries to begin to improve energy efficiency and reduce greenhouse gas emissions. For the Forest Products industry, a partnership with DOE and the subsequent publication of Agenda 2020 answered this call. Agenda 2020 specifically details research goals and objectives to aid in meeting the goals of the 1992 Energy Act within the paper industry.

The Institute of Paper Science and Technology (IPST) and the DOE have created the ‘Efficiency in Manufacturing Design Competition’ for the Forest Products industry, otherwise known as the Energy Challenge. The goal of the Energy Challenge is to increase awareness of Agenda 2020, the paper industry, and green engineering. In the past five years, competing teams have had to design and construct such diverse products as thermal and impact resistant packaging, a kayak, a sailboat sail, a sailboard, and a hang glider airfoil, all comprised of a majority weight percent cellulose fiber and all following the principles of Agenda 2020. This year, teams were expected to create a snowboard with similar design considerations.

The Red Wolf Board Company (RWBC) has designed and built a snowboard incorporating alkaline sulfite anthraquinone (ASAQ) pulping and black liquor gasification to increase pulping yield and to create substantial energy savings for a paper mill. Through theoretical modeling of an ASAQ pulp mill, the team was able to show that savings on the order of $5,000,000 per year were attainable. The board design includes three different composites developed from linerboard and vinyl/ester based resin combinations. Each composite has unique material properties which in some cases are similar to wood and steel. The RWBC used some of the most up-to-date techniques and equipment to aid in the fabrication of the product; in particular, computer-aided-design (CAD) cutting systems were used to accurately cut materials for the board. Short-cycle prototyping was utilized to quickly develop a working product comprised of ~80wt% cellulose fiber, with the inherent principles of Agenda 2020 and green engineering contained therein.

The final section of the project was the snowboard race in Winterpark, Colorado on April 3rd, 2004. The team had to race their snowboard against competing teams and give a brief presentation. The RWBC produced significant research into ASAQ pulping and black liquor gasification, which could create massive energy savings and was unprecedented within the competition. As a result, the RWBC positioned themselves in second place for the midterm, final report, video and performance (structural testing of the snowboard) categories and placed first in the presentation category. The team was awarded a final position of 5th place overall. Nonetheless, the RWBC developed the most research that was directly applicable to the forest products industry.
Carbon Dioxide Separation: High Temperature Flue Gas Adsorption

Brent Dixon, Bryan Kirkman, Jarek Karwowski, and Christy Taylor
Advisors: Dr. Lisa Bullard, Dr. Nick Hutson

Carbon dioxide is currently a non-regulated emission that accounts for up to 55% of greenhouse gases. Interest in minimizing the amount of CO₂ released into the atmosphere has prompted research by various groups. The US DOE has considered several options for reducing the emissions of carbon dioxide. One of these options is the sequestration of CO₂. This design team researched pressure swing adsorption as a method of carbon dioxide separation. Using a pressure swing adsorption unit, as an addition to fossil fuel power plants, could allow for greater than 90% CO₂ removal. The senior design team has focused specifically on designing an add-on PSA facility for the removal of CO₂ from both coal and natural gas combustion processes. A research team from the University of South Carolina, led by Dr. James Ritter, has created a basic mathematical model to simulate the PSA process. This model was used to obtain equipment sizing information and gas flow characteristics.

The efficiency of the PSA unit is directly related to the type of sorbent used in the system. After extensive research, hydrotalcite-like compounds (HTlcs) were chosen as a promising sorbent because of their high adsorption capacity for CO₂ at elevated temperatures. This material is easily modified, both chemically and physically, to increase effectiveness. Modified HTlcs exhibit an adequate working capacity, high mechanical strength, adequate kinetics for adsorption and desorption, a strong physisorption nature without significant irreversible chemisorption, and insensitivity to the presence of water vapor.

Permanent storage of the captured CO₂ from power plants to geological formations requires an efficient transportation method. Due to the large, continuous volumes of CO₂ that will be collected, pipelines provide the most promising transportation option. Using geological formations is a favored method for long-term storage because of high storage capacity and small environmental impact. These formations include depleted natural gas and oil reservoirs, unminable coal seams, aquifers, and saline formations. Saline formations are the best choices for the storage of CO₂ because they are located virtually all around the world.

The cost associated with constructing and operating a PSA facility was calculated. A cost analysis for each piece of equipment was performed, and total module costs, as well as manufacturing costs, were obtained. The capital cost associated with the additional of a PSA facility for a coal power plant is $77M and $54M for a natural gas power plant. The energy required to operate a coal power plant is 5.6 MW and 4.6 MW for a natural gas power plant; therefore, the coal power plant suffers a 22% energy penalty and the natural gas power plant suffers a 19% energy penalty. This energy penalty is above the US DOE goal of 5%; however, with improved technologies and a more in-depth investigation, this method of CO₂ capture could be feasible. The design team proposes that a pilot-scale test facility be added to an existing natural gas power plant so that a more detailed study can be completed.
Reducing the Risk of Cancer from Fried Foods

Justin Mathes, Brian Mills, Jonathan Rice, and Ravi Shah
Advisors: Dr. David Ollis, Dr. Lisa Bullard

During the last two years, new research conducted mainly in Europe has discovered the suspected human carcinogen acrylamide in a wide variety of fried foods, most notably in French fries and potato chips. This discovery is surprising, as the raw potatoes contain no acrylamide. The objective of this project is to design a system that eliminates acrylamide from French fries and chips. The major goals of this project were to work out the kinetics of acrylamide formation in these foods and to develop a wash process to reduce acrylamide precursors from the surface before frying. The surface or crust of potato chips and French fries contain the highest concentrations of acrylamide because they are exposed to the highest temperature during frying.

To reduce or eliminate acrylamide in the final fry and potato chip product, a wash process was developed to remove asparagine and glucose from the surfaces of raw potato slices and strips. The wash process is an improvement of a step already used in French fry and potato chip manufacturing. In the current system, raw potato slices and strips are rinsed for several seconds with high-pressure water jets to remove surface starch. The improvement introduced here would replace the very brief spray wash with a stagnant water bath lasting for 15 minutes. This soak will allow time for molecular diffusion to remove the water-soluble asparagine from the cut cells on the potato surface, but would leave behind most of the cells’ starch, which is responsible for much of the flavor characteristics including crust formation.

The wash process introduced here removes 95% of the acrylamide precursor, asparagine, from the top layers of potato slices with a 15-minute extraction time. This results in a 33-71% decrease in total acrylamide from each French fry depending upon the thickness of the formed crust. A kinetic rate equation was developed assuming either 2 or 3 intermediates in the formation reaction of acrylamide. By fitting the model to literature data, the value of the rate constant, k was found to be 0.399 min.⁻¹ with a lag time of 3 minutes.

The cost to implement the modified wash process is economically viable. It was found that a wash vessel capable of processing one ton of French fries per day would need to be 283 liters. Installed, this vessel costs $14,800 and can be attached to existing conveyors and water lines. The yearly operating cost assuming 24-hour operation is $3600.

However, it is recommended that these theoretically calculated results be further tested with more substantial experimental data. Experimentation should also be done to ensure that the proposed wash process does not significantly affect taste quality. Optimal frying conditions should also be determined experimentally. Using data from the kinetic model, an optimal time and temperature profile within the fryer can be found which will produce quality fries with reduced acrylamide concentration. The models are consistent with the sparse level of data available in literature, for both the extraction process (precursor removed) and the final fry process (acrylamide formation).
Currently, the preeminent method of power generation in the United States is the combustion of hydrocarbons. The United States relies heavily on combustion technology because the range of this technology is from power plant grid generation to portable power generation. Unfortunately, combustion technology results in the release of harmful toxins, which have detrimental effects on our planet and all its inhabitants. Even if combustion’s harmful effects ceased this year, there would still be permanent irreversible damage left to our planet and its stratosphere. The petroleum which is pumped from below our planet’s surface has existed there for millions of years, and by 2030 it is estimated that half of what we can easily access will be gone. Thus, there is a required change to how the United States and the world meet their energy needs.

The goal of this project is to develop a portable hydrogen fuel cell system which can compete with portable combustion power sources. The successful development of this system could be the first step in demonstrating that fuel cells can replace combustion technology. In order to realize this goal and to perform a complete quantified analysis of fuel cells, the following tasks were completed. A technical background and justification of the process were developed. This includes a discussion of the different fuels and fuel cell technologies available and provides justifications for sodium borohydride and the proton exchange membrane, which were chosen because they best fit our specifications. A block flow diagram of the process was completed. Calculations for the mass and energy balances as well as defined unit-operating conditions were also determined by hand. The proposed system was determined to weigh approximately 70 pounds and have a volume of 40 liters, with the reactor running isothermally at a temperature of 80°C. It was determined that some simple control loops would keep the system at desired conditions. A simulation of the reactor on SuperPro® Designer was also performed and confirmed that our hand calculations were accurate. In addition, all safety issues associated with the process were outlined and showed that our system, if used correctly, would be completely safe. Lastly, an economic and market analysis was accomplished. The market analysis showed that there is demand for new reliable power sources which have better properties than current combustion technologies. The economic analyses led to the realization that fuel cells and our proposed system are currently too expensive by a factor of ten for the market to accept it.

The team does not recommend that alternative power sources such as this proposed system are built or produced in the near future, although this system would effectively replace portable combustion power sources. Currently the cost associated with this system is far too great for it to realistically replace combustion power from an economic point of view. Yet, fuel cells are more efficient, reliable, environmentally friendly, and aesthetically appealing than combustion technologies. Furthermore, fuel cells are capable of supplying power at any range that combustion technologies can. Thus, it is recommended that fuel cells and PEM fuel cells are continually studied further when considering the harmful effects of using combustion technology as a means for power supply.
This report details the design of a 10 kW combined heat and power fuel cell system for Reynolds Coliseum, on the campus of NC State University. Distributed power generation with fuel cells offers many advantages over regional power generation, some of which include reduced transmission losses, increased power autonomy, and the ability to capture useful waste heat. In addition, worldwide reliance on fossil fuel is creating an air pollution problem and, as supplies dwindle, will lead to a fuel crisis. These factors necessitate research on alternative energy solutions. Fuel cells use hydrogen, which can be derived from renewable sources, as a fuel. An electrochemical reaction between hydrogen and oxygen within the fuel cell produces electricity very efficiently, and the capture of waste heat can improve total system efficiencies to over 70%.

The 10 kW fuel cell system at NC State University was designed based on performance analysis of a similar system at NC A&T State University in Greensboro, NC. The system at NC A&T is a 5 kW proton exchange membrane fuel cell manufactured by Plug Power. Funding for the system was provided by a Department of Defense (DoD) grant program. The performance analysis on the NC A&T system indicated that maximum overall efficiencies are achieved when there is full usage of waste heat generated by the system. This criteria, along with the requirements of the DoD grant, led the team to choose Reynolds Coliseum as the best site for a similar system at NC State.

The system at NC State will consist of two, identical 5 kW fuel cells with the capability to generate hot water from captured waste heat. Each fuel cell has a built-in, reformation system which converts natural gas to hydrogen for use in the cell. The total system cost is approximately $200,000, which will be provided by the DoD grant. With full funding from the Department of Defense, the cost for one kWh of electricity is 3.7¢. This is approximately half of current electric rates.

Winning a Department of Defense grant requires the proposed project to be unique. In light of this, the NCSU system was designed with several experimental purposes in mind. These include investigating the ability to vary heat to power ratio and determining the effects of this variation on fuel cell life. ASPEN software was used to model the fuel cell system and serve as a base for experiment design. The model predicts that reformer temperature and oxygen feed rate could serve as manipulated variables in a heat to power ratio control system. The identification of these variables is based on simplifying assumptions made in the ASPEN model. These include simplified reactor kinetics in the water gas shift and selective oxidation reactors.

We recommend that future design teams proceed by adding detail to the design and prepare a full grant proposal for FY 2005. This should be completed in partnership with the NC Solar Center, which will be the official applicant for the grant and will be responsible for data collection and analysis.
This project involved the construction and validation of a computer model of an existing pilot gasification unit located in Grinnells Lab at North Carolina State University. The pilot unit is a continuous feed downdraft steam reformer, used in the study of swine feces conversion to synthesis gases including H₂, CO₂ and CH₄. The primary goal of the project was to develop and validate an experimentally based simulation of the biomass gasification process using SuperPro® Designer, and analyze the effects of varying feed composition, temperature, and pressure on the reaction products. The secondary goal of the project was to design the scale-up of the biomass gasifier pilot unit to a plant that produces synthesis gas from hog waste.

The SuperPro® model was constructed to handle a range of temperatures, pressures, and feed compositions: 750-950°C, 100-200 psi, and 70-80% dry weight of feed. Any combination of these parameters will result in a unique array of product gas amounts and compositions. The validation of the model has been somewhat compromised due to the fact that only two experimental runs produced adequate results available for analysis. The product gas amounts produced by the model are similar to those observed experimentally. The overall product gas amount produced by the model is 10.4% greater than the amount observed experimentally. This is due to the greater amount of ash and tar observed experimentally (5.92 kg) than the amount simulated by the model (4.05 kg). The more ash and tar that are produced, the less material available for conversion into synthesis gas. The differences between the model and experimental percent compositions of the product gas are less affected by the discrepancy in ash and tar production because the comparison does not depend on the overall product gas amounts. The percent differences between the mole percentages of CO, H₂, and CH₄ in the model and those observed experimentally are less than 5%. Overall, the model accurately predicts the amounts of product gases at the conditions tested. The results of the analysis of product gas flow rates with changing reactor conditions, agreed with the relevant chemical principles. From the analysis of the trends, the optimal system setting would be 950°C, 100psi, and 70% dry weight of feed.

The SuperPro® model was scaled up to incorporate a 250 ton/day feed rate. The total capital costs were approximately $5 million and the manufacturing costs were approximately $9 million. The gasifier plant itself would have revenue from the sale of ash to fertilizer companies of $500,000. This amount does not come close to making the plant profitable. The most feasible method of turning a profit would be to build an adjoining plant that converts the synthesis gas into ethanol, which has estimated annual revenue of $29 million.

Based on the analysis of the gasifier model, it is recommended that more experimental runs be made on the Grinnells gasifier at a wide range of parameter settings in order to achieve a more accurate model. This would cause the uncertainty in the model to significantly decrease. Concerning scale-up, a more thorough design should be made of the gasifier plant and an additional design should be made of the adjoining ethanol plant to fully realize the feasibility of such a venture.
A high-grade gelatin manufacturing plant in North Carolina has significant potential in terms of financial return from an abundant supply of raw materials in the state, as well as a growing regional market of biotechnology and pharmaceutical industries. These expanding North Carolina businesses are demanding a higher quality gelatin than currently available, primarily for application in medical devices. A medical device is any physical item used in treatment, such as an injected wound dressing. Gelatin is a key component in these devices and must meet strict purity standards before the medical device can be guaranteed safe. Biotech and pharmaceutical companies will pay top dollar for a gelatin that can be certified safe.

A computer-generated model of the proposed plant using SuperPro® software illustrates and models the entire production process, including waste treatment, quality, and safety control. An economic analysis of the proposed plant indicates that operating costs will be approximately $3.85 million per year and the total capital investment is approximately $10.04 million. Currently, North Carolina ranks second in the nation in pork production generating about 75 million kilograms of skins annually. If 224,000 kilograms of these skins are processed to make 10,000 kg of high-quality gelatin per year, this plant could potentially generate annual revenues exceeding $10.15 million to benefit North Carolina’s economy. Based on the costs and revenue given, the payback period would be 2.15 years, a time period that clearly illustrates the feasibility and financial attractiveness of the proposed plant.

The process modeled in SuperPro(R) was verified and optimized using a bench-scale model of the extraction. Pig skins were ground, and then acid-extracted using nine combinations of time and temperature. Optimal extraction conditions of 90 °C and 20 minutes at the maximum temperature were determined based upon the yield and gel strength of the experimental gelatin samples. The proposed acid extraction process produces gelatin with a yield of 94.5 grams of gelatin per kilogram of raw material, and a relative strength ratio 1.09 compared to the target gelatin. These results verify that the proposed extraction method will produce gelatin with the required properties.

The preliminary research contained within this report leads to the recommendation that resources be spent to further investigate the proposed gelatin plant. Further research should include evaluating the effectiveness of the endotoxin removal procedures and re-evaluating the annual production rate by constructing a more detailed estimate of the demand for medical grade gelatin.
The Kennametal plant located in Henderson, North Carolina, is a leading producer of tungsten carbide metal power, which is used in the making of inserts for cutting tools. The tungsten carbide production process begins by heating tungsten oxide raw material to rid it of its ammonia impurities. The purified tungsten is then blended with carbon powder to fabricate a durable product. Once equipment is washed, the wash water proceeds to a sump where any residual product can be recovered. The heavier tungsten carbide particles settle and the process water discharges to the city sewer. The plant has a history of contaminant exceedances in its process water effluent. Contaminants include zinc, copper, total Kjeldahl nitrogen (TKN), pH, methylene blue active substances (MBAS), and chemical oxygen demand (COD). Process water comprises regularly scheduled boiler blowdowns, recirculating water bleed-offs, wash-downs of milling equipment, and water of hydration generated by the heating of raw tungsten oxide.

Lab testing of wastewater samples taken from various plant processes determined the sources of each contaminant. The blowdown, bleed-off and sump effluents were the primary contributors to zinc and copper concentrations. The ammonia impurities removed from the raw material result in high TKN concentrations and the soaps used to clean the equipment were responsible for the high MBAS and COD concentrations. Process changes and treatment options were considered to reduce or eliminate these concentrations. Investigated upstream process changes include lining or replacing pipes, closed loop inhibitors, recycling treated wastewater, and cleaning alternatives. Downstream wastewater treatment options that were explored include air stripping, flocculation/sedimentation, filtration, carbon dioxide diffusion, reverse osmosis and ion exchanger.

Implementing several of the upstream process changes entails shutting down production and possibly replacing significant amounts of equipment and piping, making these options uneconomical. For example, lining of pipes is a temporary solution to the corrosion of metals; however, the piping would ultimately need to be replaced. As a result, downstream water treatment options are recommended to mediate Kennametal’s violations. The ammonia-rich wastewater stream should be treated separately from the other process water streams due to interferences by ammonia on metal solubilities. Once isolated, the ammonia-rich stream should be treated via air stripping. The remaining streams should be treated using a flocculation/sedimentation system with the option to include filtration if sedimentation cannot adequately reduce metal concentrations to meet City limits. After these processes are complete, carbon dioxide diffusion should be used to lower the pH of all wastewater streams to within the permissible range of between 6 and 10. These recommended processes will produce a wastewater effluent that will be in compliance with the various pollutant limits set forth by the City of Henderson.
This report proposes a treatment process for medical waste generated in underdeveloped areas, including some parts of rural America and undeveloped nations. According to the World Health Organization, there is a need for a low cost, low tech process that can successfully treat medical waste in these areas. Current technologies for treating medical waste include a number of methods such as, incineration, steam or gas sterilization, thermal inactivation, and chemical disinfection. However, these areas currently lack the money, expertise, and resources needed to facilitate many of these processes. As such, poor sanitation and living conditions are presenting problems for everyday life in these areas. A set of criteria and constraints were developed in order guide the modeling of a process that could possibly meet the treatment needs and feasibility requirements of these underdeveloped areas. The most important aspects of the criteria include non-burn technology, safe operation, minimum environmental impact, ease of manufacture, and the ability to treat a range of medical waste streams. The remaining criteria were used as design constraints.

Through careful analysis of the current technologies, chemical disinfection was chosen as a feasible means of medical waste treatment due to its ability to meet the project constraints. This process allows for flexible implementation and depends heavily on the chemical chosen. The chemical must be safe to use, possess disinfection capabilities, and present minimal disposal concerns. A number of different chemicals were evaluated in order to meet the constraints, including hydrogen peroxide, ammonia, glutaraldehyde, lime, isopropanol, and ethanol. The chemical best suited for use in these areas was ethanol due to its status as a good disinfectant, low cost, safe use, biodegradability within the environment, and local production capability.

In order to be considered a good disinfectant, the ethanol must produce a 4log_{10} reduction of bacteria (99.99% kill) when treating medical waste. Research shows that 70 volume percent ethanol concentration can achieve a 4log_{10} reduction in as little as ten minutes; however, in order to ensure that ethanol has reached the medical waste in its entirety, it should be soaked in ethanol for no less than three hours. Seventy percent ethanol is considered the most effective concentration for disinfection and is recommended for this process. The maximum capacity of the process is 41 kilograms. This means the average batch of medical waste generated each day, ten kilograms, can be easily accommodated by the design. A cost analysis of this process reveals that implementation will cost approximately $1500 in the first year and approximately $1300 annually in subsequent years. This is significantly less expensive than many current technologies and could be economically feasible to most underdeveloped areas. Further experimentation could determine if lower concentrations of ethanol will produce a 4log_{10} kill of bacteria and the extent to which ethanol can be recycled, further reducing operating costs.
Microfluidic Cooling Device for Microprocessors

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Microprocessors are advancing faster than the development of the corresponding cooling technology. Currently available heat sinks are adequate for the present cooling needs, but are ill-suited for the demands of tomorrow. Microfluidic technology is a possible solution for removing the increasing amount of heat generated by microprocessors.

The Microfluidic Design Group has designed a microfluidic heat sink for the specific purpose of removing 300 W from a microprocessor. A state-of-the-art microfluidic device, utilizing a coolant undergoing a liquid-vapor phase transition, was designed. The cooling device consists of a heat sink with microchannels, a vapor chamber, fins with microchannels, fans, a liquid reservoir, and micropumps. The heat sink will be positioned directly above the microprocessor. The coolant (water) will be pumped by electroosmosis into the heat sink channels. As the coolant flows across the heat sink, it will vaporize as heat is being transferred from the microprocessor. Most of the heat dissipation will take place during the phase change; therefore, a coolant with a high heat of vaporization was chosen. The microprocessor temperature will approximately correspond to the boiling point temperature of the coolant, which in the case of water is 100°C. The water vapor coming out of the heat sink will be directed to a vapor chamber and will then flow to the microchannels in the fins. The vapor flowing in the channels in the fins will condense as air is blown across the fins by two fans. The condensate coming out of the fins will then be collected in the liquid reservoir and pumped back into the heat sink. This completes the two-phase liquid cooling cycle.

The benefits of the microfluidic cooler design proposed by the Microfluidic Design Group are:
- Power efficiency, removing 300 W while using only 14 W
- An inexpensive, safe and readily available coolant (water)
- Economy of size; the heat sink is smaller than a brick
- Inexpensive and simple construction from plastic and copper parts
- No maintenance and high reliability: closed system with no moving parts

The design was based on the assumptions that the Homogeneous Model accurately describes the pressure drop of the system; the system remains at steady state; and the heat sink base has a uniform temperature profile. Calculating precisely the fluid dynamics inside the microfluidic device is currently a limitation that could be addressed in the future. Despite this limitation, the Microfluidic Design Group has proved that the design of the microfluidic cooling device has the potential to meet future heat dissipation needs.
Perchlorate Treatment for Domestic Water Systems

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Perchlorate contaminated groundwater is a problem currently plaguing the Western United States. The majority of perchlorate contamination is a direct result of the manufacturing and testing of solid rocket fuels. The state of California is setting the standards in perchlorate regulations, setting a 4ppb maximum concentration level for potable water.

The scope of this project was to design and construct a bench scale perchlorate removal system that could be implemented in a water treatment facility (WTF). Also, to design a WTF and distribution system, to remove several contaminants provided by the WERC, including perchlorate, down to potable water standards for a 200-person community in Pasadena, California.

There are two methods available for perchlorate removal, abiotic and biotic. Abiotic methods remove perchlorate via chemical or physical means. Biotic technologies employ bacteria to degrade the perchlorate to chloride and oxygen. A biotic fluidized bed reactor (FBR) was chosen as the perchlorate treatment method.

The bench scale team constructed the FBR in January, and after inoculating the reactor with bacteria, began running experiments in mid-February. The first phase of experiments ran for 48 hours each; it was discovered that 48 hours was not a sufficient amount of time to allow the reactor to reach steady state behavior. The second phase of experimentation began in mid-March; this experiment ran for a total of 3 weeks to allow the reactor to run at steady state conditions. Results from the second experiment show the reactor was degrading perchlorate to below the laboratory’s detection limit of 50ppb, proving that the biotic FBR system was a viable means to remove perchlorate from contaminated water.

The scale up team designed the WTF to purify the water described by the WERC in early January. The WTF design includes several unit operations, including the scaled-up biotic fluidized bed reactor constructed by the bench scale team. The facility capital cost would be approximately 1.6 million dollars, with a yearly operating cost of approximately 0.7 million dollars.

The recommendation of the team is to not implement the designed WTF for a 200-person community because of the high cost associated with the plant. To minimize cost, the Reverse Osmosis (RO) system included in the WTF could be used to remove the perchlorate in the source water. However, this will produce a hazardous waste stream. Another alternative is to implement a biotic packed bed reactor system instead of the FBR system. This option decreases the high capital cost associated with the FBR system, and does not have the hazardous waste problem that the RO system produces.
The Biological Production of para-Hydroxybenzoate

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Everyday, people use products such as cosmetics, skin care, medications, electronics, and food that contain a compound called para-Hydroxybenzoate (PHBA). PHBA is either used as a preservative or as a monomer in the production of liquid crystal polymers. PHBA is produced today by a chemical process called the Kolbe Schmitt reaction. Even though this process works, there are problems: occupational concerns from high temperatures and pressures and heavy emissions of harmful substances like carbon dioxide. One way to alleviate this problem is to research and design a biological process for the production of PHBA. The goal of the PHBA Team is to develop and simulate a “green” alternative to traditional production, the Kolbe Schmitt reaction, of PHBA through a biological route and to analyze the economic feasibility of the process. This “green” alternative operates at safer conditions, and produces less harmful emissions, making it more environmentally friendly.

The design of the biological production process starts by taking a small culture of the bacteria, Pseudomonas putida, and growing it to a dense population using glucose as the substrate, a nutritive source. Once the bacteria are grown, the substrate is changed from glucose to toluene. As soon as toluene is introduced, a conversion from toluene to PHBA begins through a metabolic reaction sequence known as the TMO pathway. As PHBA is produced, it is separated from the mixture and purified. The design of the biological process includes three seed fermenters, a production fermenter, two microfiltration units, an ultrafiltration unit, a packed bed adsorption chromatography unit, a storage tank, and a crystallizer. The seed fermenters and production fermenter grow the bacteria; however, the change of substrate occurs in the production fermenter allowing PHBA to be produced. The microfiltration, ultrafiltration, and the packed bed adsorption chromatography units separate PHBA from the bacteria and other substances. The PHBA is further purified and crystallized in the crystallizer.

Currently, PHBA is produced at a rate of 19,500 tons per year. The biological production facility that has been designed produces 54360.90 kg of PHBA per batch in 34.1 hours. A total of 781 batches can be processed every year, resulting in a production of 4680.66 tons of pure PHBA per year and a 24% capture of the market. In addition, the total cost of expenses is $51 million per batch, while the total revenue per batch is $297,289.37. Since the total expense outweighs the total revenue, this biological process is economically infeasible. In conclusion, this biological route to PHBA is physically possible, but is not economically feasible.

In order to make the biological production of PHBA economically feasible, more research into the optimization of the process is required. If the amount of glucose and air, the two substances used in the largest quantities, could be reduced while producing the same amount of PHBA, the process would become more economically feasible. In addition, the system would be more cost effective if less equipment could be used. Due to the occupational and environmental concerns of the current production of PHBA, continued research of the biological production is necessary.
Thermochemical Processing of Tobacco to Produce Methanol: A North Carolina Facility

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This report proposes an alternative process for the production of methanol based on tobacco gasification in North Carolina, as opposed to the current natural gas method. The primary motivation for this project is to use a renewable resource to produce a gasoline alternative in the automobile industry. It is estimated that the world’s oil reserves will be depleted in approximately 40 years, and renewable sources of energy must be developed. A faster shift away from petroleum products could also free the United States from international oil prices. Other motivators are the possible revitalization of the North Carolina tobacco industry, which has been in decline since 2001, and the mitigation of atmospheric CO₂ accumulation that comes with biomass production.

The facility processes 2500 kg of tobacco per day, about 4% of all North Carolina flue-cured tobacco, and produces 1180 kg of methanol per day. The tobacco is first shredded and partially combusted in a fluidized bed reactor. The gaseous products are sent to 4 plug-flow reactors where they are converted to methanol in a catalyzed reaction. The methanol is then purified to 97% using distillation columns. The computer simulators Microsoft Excel®, MatLab®, and SuperPro® were used to model the reactions.

The largest limitation on future implementation of this process is that the feed, tobacco, is currently much more expensive than the methanol product ($4.04/kg and $0.25/kg, respectively). The operating costs of the facility, including the costs of raw materials, exceed $94M per year, as calculated by SuperPro®. Revenues from methanol generate $2.3M per year. This price discrepancy results in a large negative rate of return on investment of -337%. Another factor which increases facility and operating costs are the large sizes of methanol reactors. The four reactors constitute over half of all equipment costs ($2.4M). Their large size is due to poor one-pass conversion (5%) which results in recycle streams. Low-one pass conversion of the synthesis gas due to catalyst efficiency is a problem that could be addressed to reduce reactor residence time and size.

Studies have shown that the gasification of other feedstocks, including wood, straw, and even municipal waste, can produce similar amounts of gas to synthesize into methanol. This is promising, because most of these feeds cost less than tobacco. Industrial waste biomass could also be used, and the methanol plant could receive revenue by removing the unwanted biomass waste of other industries. Government incentives are also available for industries involved in renewable fuel production, and these could help make the use of such a facility more realizable. The environmental benefits and the potential in aiding the tobacco industry in North Carolina do not currently outweigh the large financial losses associated with the facility, and it should not be built. The implementation of renewable energy facilities is necessary, however, and such a facility could become economically sound in the near future.
Currently, there are approximately 1 million people suffering from AIDS Wasting syndrome and cancer-induced nausea and vomiting (CINV). Presently, Marinol®, an oral medication containing synthetic THC, is prescribed as an anti-emetic and appetite suppressant. Although Marinol® users benefit from avoiding the dangerous tars found in smoking medical marijuana, the oral form has several disadvantages. The drug takes roughly an hour to take effect, and those taking the pill as an anti-nausea remedy have a difficult time even keeping it down. Therefore, a unique opportunity exists. An inhaled formulation of THC would provide the quick action of smoked marijuana (approximately 3 minutes) without the harmful effects of inactive chemicals such as tar.

A relatively new technology, known as RESAS (Rapid Expansion of Supercritical Solution into Aqueous Solution) has been found to create particles on the order of 450 nm in diameter, ideal for delivery through a nebulizer. Based on the potential marketability of a new formulation of THC, the goal of this project became the development of a suitable RESAS process that would produce 40 kg THC per year, the equivalent amount that would treat those that would currently take Marinol®. In addition, the process was evaluated for its expandability to higher production rates and flexibility for other product materials. The process utilizes supercritical CO₂, a material found abundantly in nature that is nontoxic, and inexpensive. The use of supercritical CO₂ as a solvent has gained much acclaim in this era of “green engineering”, as it is much less toxic that conventional solvents, and also requires little to no processing before environmental release, thereby reducing treatment costs.

A daily output of 146 g THC in solution, stabilized with Tween-80, is achieved through a 4 hour batch process. A tank is initially charged with CO₂ and Tween-80 in aqueous solution. The process then runs as a loop. CO₂ is compressed to a supercritical state, in which THC is dissolved to form a solution. This solution passes through a nozzle into a sub-critical vessel, precipitating out the THC in micronized particles. These particles are stabilized by the Tween-80. CO₂ is recycled through the loop, reducing raw material costs. The fixed capital investment for this process was calculated to be $94,164. Raw material costs accounted for 56% of the annual operating costs, with THC and CO₂ comprising 48% and 7% of the annual operating cost, respectively. For this process to be feasible, it is imperative to find a less expensive source of THC, since nearly half of the yearly expenses are the purchase of THC.
Acme Biotechnology, Inc. has issued a project analyzing options to increase productivity for the fermentation and recovery processes of Binding Protein #01 (BP1). This particular binding protein is used by other manufacturers to produce polysaccharide-protein conjugates, which are used in the production of conjugate vaccines. We were asked to model the current process using material balances, and compare our results to those found using the SuperPro® simulation package. This comparison will be used to provide a basis for computer modeling standards, and to verify that SuperPro® is an accurate process simulator. A User’s Manual and training materials were developed to support ACME in future process optimizations. Using the simulated process as our base standard, we were asked to improve the process by analyzing two different types of fermentations and performing productivity optimization.

Phase I involved the completion of a general process description, which was used to define information for SuperPro® modeling purposes. Subsequently, the general process was modeled in SuperPro®, and the simulation specifications for the User’s Manual were outlined. Meanwhile, material balances were performed on all unit operations in the fermentation, recovery, and purification processes. These calculations aided in the further specification of the operating conditions for the production of BP1 and to validate SuperPro®’s results.

Phase II saw the completion and evaluation of the process through SuperPro®, including: environmental impact analysis and economic evaluations. The simulation results were compared to the manual calculations to validate the operational capabilities of SuperPro®. SuperPro® results were found to be consistent with the results calculated manually, and the economic evaluation of the simulation provided proof that the process results were economically feasible. After validating SuperPro®’s results, construction of the User’s Manual commenced, beginning with modeling standards, general formatting, and layout. Construction on the User’s Manual then proceeded to elaborate on simulation topics such as inputting simulation data, setting operations and establishing unit procedures. Meanwhile, research was conducted for two different fermentation opportunities: fed-batch fermentation and plasmid insertion. The focus of this research was centered primarily on the current technology behind each option and the associated advantages and disadvantages.

During Phase III, User’s Manual development proceeded by incorporating all functions necessary to simulate a bioprocess in SuperPro®, as well as an extensive index for aiding in the navigation, through the manual. In addition to the User’s Manual, further research into the optimization options was performed, and SuperPro® aided analyses were completed to determine the pros and cons of each option. It was found that both fed-batch fermentation and plasmid insertion could reduce the time required for fermentation. Finally, economic analysis proved that plasmid fermentation is the most profitable and feasible alternative.