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Developing models for analyzing cost structures in fermentative bioprocesses

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Developing models for analyzing cost structures in fermentative bioprocesses

by

Carol Faulhaber

A thesis submitted to the graduate faculty

In partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Co-majors: Agricultural and Biosystems Engineering; Biorenewable Resources and
Technology

Program of Study Committee
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Ames, Iowa

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ABSTRACT

The main objective for this thesis was to develop techno-economic modeling tools to analyze two bioprocessing systems: anaerobic digestion and industrial fermentation. While both of these processes can be used to produce products that ultimately offset fossil fuels, there are fundamental differences between each process. Anaerobic digestion is a mixed culture process used for waste treatment – it uses a feedstock of low or sometimes negative value. In contrast, industrial fermentation is a pure culture process typically used to create high value products, requiring relatively expensive feedstocks and typically higher-technology infrastructure to support. Understanding the cost structures of different bioprocesses helps engineers and scientists identify critical variables that should be targeted for reducing production costs. This thesis is prepared in the journal paper format and includes two papers that have been prepared for submission to a journal.

The objective for the first paper in this thesis was to develop a model to analyze farm-scale anaerobic digestion. Anaerobic digestion is a biological process that can be used to treat animal waste, producing biogas and a nutrient-rich digestate. A spreadsheet model was developed to analyze economic and technical barriers to this technology, using operation size as the primary input and the cost for producing methane as the primary output. Trends in the methane cost ratio, or the ratio of the production cost for methane to the market value of natural gas, as a function of different process variables were evaluated, and recommendations for improving deployment rates were discussed. Results showed that moderate reductions in the interest rate are capable of making 1000-cow digesters economically feasible if high carbon credits values, high natural gas prices, and low gas clean-up costs can be achieved;

however, if carbon credit values are low as they currently are, more extreme modifications to the digester cost and interest rate, combined with increases in digester life and/or natural gas prices are required for smaller dairies to break-even when using anaerobic digestion.

The objective for the second paper was to develop a model to analyze the cost structure of industrial fermentation processes for producing biorenewable chemicals. As metabolic engineers develop improved microbial strains for industrial fermentation, understanding the tradeoffs between different kinetic parameters on the production cost is vital. A spreadsheet model was developed to provide an order-of-magnitude estimate of chemical production cost based on kinetic and operating parameters. Results showed that production cost is most sensitive to yield, fraction of product in the biomass, and substrate concentration. Feedstock cost makes up the largest portion of the production cost except under the most pessimistic fermentation conditions. Minimizing fermentation costs is critical to making biorenewable chemicals cost competitive with their well-established petroleum-derived competitors.

CHAPTER 1. GENERAL INTRODUCTION AND REVIEW OF LITERATURE

Fermentative bioprocesses date back to 6000 BC and have been utilized for food, beverage, energy, and chemical production throughout history (Scragg, 1988). After Anton van Leeuwenhoek discovered the existence of microorganisms in the seventeenth century, the field of biotechnology emerged as scientists learned how to harness and manipulate microbes to develop pharmaceuticals, chemicals, food products, and biofuels (Scragg, 1988 and Cooney, 1983). As the Industrial Revolution progressed, industry shifted its focus to fossil-based resources for chemical, fuel, and energy production with the discovery of an inexpensive feedstock, oil. The 1970's oil crisis sparked a renewed interest in bioprocessing as the world recognized the finite and limited nature of fossil fuels; however, the challenge of developing bioprocesses that could compete economically with inexpensive fossil fuels hampered wide-spread deployment.

This thesis evaluates two different bioprocesses—farm-scale anaerobic digestion and industrial fermentation for biorenewable chemical production. While both of these processes can be used to produce products that ultimately offset fossil fuels, there are fundamental differences between each process. Anaerobic digestion is a mixed culture process used for waste treatment, and it uses a feedstock of extremely low (or even negative) value. In contrast, industrial fermentation is a pure culture process typically used to create high-value products, requiring relatively expensive feedstocks and typically higher-technology infrastructure to support. Each technology is explained in further detail below.

Anaerobic Digestion

Anaerobic digestion (AD) is a multiple stage process that utilizes bacteria to decompose organic waste such as manure in an oxygen-free environment (Speece, 1996). Hydrolysis and fermentation, the first stage of anaerobic digestion, converts complex carbohydrates to monosaccharides. Acidification, the second stage of AD, involves acetogenic bacteria that further degrade complex molecules in preparation for methanogenesis. During this stage, acetate and the hydrogen and carbon dioxide released during the previous stages are converted to methane and carbon dioxide (Speece, 1996). The gas released during AD is referred to as “biogas” and can be directly used for heat, used in a generator to produce electricity, or purified to produce pipeline-quality natural gas (USDA NRCS, 2007). Another co-product of AD, digestate, contains minerals and nutrients beneficial in crop production and can be land applied as fertilizer (USDA NRCS, 2007). Additional benefits of this process may include odor reductions in the digestate and reductions in manure pathogenicity (Yiridoe et al., 2009). Despite the benefits of AD there are several challenges that have inhibited technology deployment in the US.

AD was first utilized at an industrial scale in Bombay in 1859; however, the mechanisms and conditions for anaerobic growth and biogas production were not understood until the 1930’s (Monnet, 2003). As our understanding and knowledge of AD increased, the technology was further developed to process diverse waste streams. The US adopted AD for use in municipal sewage treatment plants during the 1940’s and after World War II many other countries followed suit, using AD to generate a renewable fuel source and offset power generation costs (BC Ministry of Agriculture and Land, 2009). Interest in AD intensified

during the 1970's as a result of the oil crisis and manure-fed digesters were installed in the US and abroad. Between 1970 and 1990, approximately 70 farm-scale digesters were installed in the US; however, most of these are no longer in operation (USDA, 2008). Alternatively, Europe has seen tremendous growth in AD technology and 5,000 digesters are currently installed with another 15,000 expected by 2015 (BC Ministry of Agriculture and Land, 2009). This difference in growth may reflect government policies, differences in local resource and energy availability, and differences in the cost of energy. With increasing pressure in the US to identify renewable fuel sources and reduce our environmental impact, farm-scale AD is once again receiving serious attention from policymakers. The US Secretary of Agriculture announced an agreement with US Dairy Producers in December, 2009 to reduce Greenhouse Gas (GHG) emissions from dairy farms by 25% before 2020, citing AD as the primary method for accomplishing this task (USDA, 2009). To achieve the deployment rates required to meet this goal, we must first understand the current state of anaerobic digestion and why operations have failed in the past.

According to the US Environmental Protection Agency's (EPA) AgSTAR program, 151 digesters were in operation as of May 2010 (AgSTAR, 2010). Of these digesters, the majority are plug-flow digesters. In addition, 82% of the digesters utilize dairy manure as the primary feedstock (AgSTAR, 2010). Plug flow digesters are typically the least expensive type of digester, are simple in their design, and can be used for concentrated dairy manure streams (Burke, 2001). Based on these factors, farm-scale plug-flow digesters utilizing dairy manure as the primary feedstock are the main focus of our study.

The hypothesis of our work is that the ratio of the AD methane production cost to the market natural gas price is an indicator of deployment rates for the technology. If this ratio, which we give the term, “Methane Cost Ratio” or MCR, is greater than one, the production cost is too high and farmers are less likely to operate digesters. However, MCR rates of one or less than one illustrate scenarios when AD is economically competitive and times when we would expect to see higher deployment rates. The key concept behind MCR is return on investment. The University of Missouri completed a focus group study to analyze barriers in precision agriculture and found that the most important factor to producers was cost (Wiebold et al.). When farmers talked about cost during the focus group, they mentioned the capital cost, time required to effectively implement the technology, and the return on investment (Wiebold et al.). While anaerobic digestion is a different technology within the agricultural sector we believe that the same principle of return on investment still applies. For producers to implement AD, they expect to benefit from using the technology financially. In the case of AD, return on investment can also include non-monetary benefits such as odor reduction and GHG emissions reductions. These factors were also quantified and incorporated into the model as potential “credits” that AD might receive with appropriate policies.

Industrial Fermentation

While brewing was developed by the Sumerians in 6000 BC and other fermentation processes for making bread, cheese, and vinegar were introduced around 4000 BC, biotechnology and large-scale industrial fermentation for the production of chemicals only emerged in the early 1900s (Scragg, 1988). One of the first industrial fermentations was

acetone butanol (AB) fermentation. The process, developed by Weizmann in 1912, utilized *Clostridium acetobutylicum* to produce acetone, butanol, and ethanol from starch (Ezeji et al., 2004). This process became critical during World War I for the production of cordite, a smokeless powder used in ammunition (Jones and Woods, 1986). After the war, AB fermentation continued to develop and was used in the automotive industry for producing solvents for quick-drying lacquers (Jones and Woods, 1986). AB fermentation expanded rapidly and new feedstocks and microbial strains were developed to increase yields and utilize glucose-based feedstocks in addition to starch. By the 1950s the primary feedstock for AB fermentation in the US was molasses. During the 1950s, the market value of molasses rose and competition increased with the petrochemical industry, leading to the decline of AB fermentation (Jones and Woods, 1986).

The history of AB fermentation is a prime example of the importance of economics in industrial fermentation. AB fermentation could not withstand the economic pressures that arose from the petrochemical industry due to the low cost of fossil-based fuels. While, the 1970s oil crisis brought about a renewed interest in industrial fermentation and biorenewable chemical production (Qureshi and Blaschek, 2000), the issues that led to the decline of AB fermentation are still challenges that must be overcome. In the past 30 years, technologies have developed to aid in this effort (Nikolau et al., 2008).

With the invention of genomic sequencing, the field of metabolic engineering developed to study genomic data to better understand the structure and regulation of organisms on the genetic level (Nikolau et al., 2008). With this information, metabolic engineers have been able to transform the genetic makeup of organisms, improving yields,

productivity, and titer in fermentation processes, and enabling microorganisms to withstand environmental conditions that they previously could not survive in. As metabolic engineers develop new microbial strains, understanding the cost structure of fermentation processes and the impacts and tradeoffs between kinetic parameters is critical. Numerous studies have evaluated the economics of different fermentation processes and several software programs are available for process design and economic analysis (US DOE, 1993; Shanklin et al., 2000; Qureshi and Blaschek, 2000; Akerberg and Zacchi, 2000).

One study that set the stage for research in biorenewable chemical production was completed by the DOE in 1993 (US DOE, 1993). The DOE developed a screening methodology to rank various chemicals based on potential biochemical production routes. The ranking calculation was based on the cost of the feedstock and the value of the products based on the theoretical yield and risk. While this method is good for identifying chemicals that would potentially be economically feasible, a new level of analysis is needed for metabolic engineers to better understand how their contributions impact the economics of industrial fermentation.

On the other-hand, detailed process models are also available to use for industrial fermentation analysis. Two common software packages on the market for industrial fermentation modeling include Aspen Batch Plus and Intelligen SuperPro. In each program, the user creates a process flow diagram and then characterizes different states throughout the process. The program then completes energy and material balances for the process and can be used to evaluate scheduling options and economic data (Shanklin et al., 2000). While these programs help engineers determine the costs for a project or optimize a process

schedule, they require several inputs and are therefore not suitable for first-level approximations to understand tradeoffs between kinetic variables. Several researchers have also developed specific process models to better understand economic tradeoffs. Qureshi and Blaschek (2000) developed a spreadsheet model to analyze butanol fermentation. While Microsoft Excel provides a good platform for techno-economic analyses as it is commonly available on windows computers, Qureshi and Blaschek's model required several process specific inputs, incorporating grain processing, fermentation, and recovery into the model. In addition, process-specific energy and material balances were used to add further detail to the model. While these detailed calculations are necessary in design work, our goal was to understand tradeoffs between kinetic variables to provide metabolic engineers with the data necessary to understand the economic impact of different genetic manipulations. Another model developed by Akerberg and Zacchi (2000) incorporated a kinetic and cost model to analyze lactic acid production cost. Using kinetic data creates a more dynamic model; however, as with Qureshi and Blaschek's model, Akerberg and Zacchi analyzed every step in the process from liquefaction to electrodialysis. These models incorporate so much detail that they mask trends in the overall cost structure and discourage economic analyses early in the design process.

Based on the models available for analyzing bioprocesses, there is a need for a simpler model that can be used early on in the research and development stages and incorporates kinetic parameters and economic data to predict trends in the cost based on experimental data.

Objectives

The research objectives for this work were as follow:

- To develop a spreadsheet model to analyze farm-scale dairy plug-flow anaerobic digestion
- To provide recommendations to improve AD deployment rates
- To develop a spreadsheet model using simple kinetic parameters to estimate the cost for producing biorenewable chemicals
- To analyze trade-offs between substrate concentration, maximum specific growth rate, separation costs, and the fraction of the product in the biomass on fermentation production cost.

Thesis Organization

This thesis contains a general introduction and literature review, two research articles, a general conclusion, and appendices containing specific modeling code and data. Included in the general introduction is a review of the literature for anaerobic digestion and industrial fermentation, the objectives for this project, and the author's role in each article.

The first article, entitled "Development of a simplified framework for analyzing low deployment rates of Farm-Scale dairy plug-flow anaerobic digestion," was submitted to the *Transactions of the ASABE*. This article makes recommendations for improving anaerobic digestion deployment rates and discusses the cost structure of digestion systems on farms. The second article, "Fermentation modeling: kinetics and the bottom line," will be submitted to *Biotechnology and Bioengineering*. This article discusses the cost structures of

fermentation processes and tradeoffs in cost resulting from different kinetic variable combinations. The references for each section are at the end of each chapter.

Author's Role

The primary author, with the support and guidance of the co-authors composed all of the articles presented in this thesis. In addition, the code and interface for each model was developed by the primary author with the guidance of the major professor.

Dr. D. Raj Raman (Associate Professor, Department of Agricultural and Biosystems Engineering, Iowa State University) conceived the original idea for the model in the first paper and provided guidance in the development of the model for the first paper. Dr. Robert T. Burns provided feedback on the model throughout development and assisted in writing and editing the paper.

Dr. Raj Raman conceived the original idea for the model described in the second paper and provided guidance in developing the interface for the model. Dr. Jackie Shanks, Dr. Robert Anex, and scientists at Grain Processing Corporation provided feedback on the model and its utility in metabolic engineering.

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CHAPTER 2. DEVELOPMENT OF A SIMPLIFIED FRAMEWORK FOR ANALYZING LOW DEPLOYMENT RATES OF FARM-SCALE DAIRY PLUG-FLOW ANAEROBIC DIGESTION

A paper submitted to *Transactions of the ASABE Journal*

C. R. Faulhaber, D. R. Raman, R. T. Burns

Abstract

Treating animal wastes through anaerobic digestion (AD) yields methane-rich biogas that can be used for power generation or heating, and a nutrient-rich digestate that can be land applied as fertilizer. Furthermore, AD reduces odors from stored and land applied manures. Despite these benefits, AD deployment rates in the United States (US) are only 5% for dairy farms identified as being suitable for AD by the US Environmental Protection Agency. The objective of this study was to analyze the economic and technical limitations of farm-scale anaerobic digesters using a simple model permitting insight into the fundamental constraints on the technology. A model was developed to determine the cost of methane produced via AD based on operation size. Dairy plug-flow systems were modeled because of their well-documented economic performance, and model validation used data from AgSTAR's Farmware program. The analysis shows how critical farm size is to making digestion-derived methane cost-competitive with natural gas. At low herd sizes (below 400 animals), carbon credits and odor reductions alone appear insufficient to overcome the low commercial energy rates in the US. However, moderate reductions in digester cost and interest rate, coupled with moderate increases in amortization period, and/or natural gas

prices could make AD more competitive with commercial energy in the US even at relatively small herd sizes (ca. 400 animals).

Introduction

Anaerobic digestion (AD) is a biological process that converts a portion of the organic material in a waste stream to biogas and produces digestate that can be land-applied as fertilizer (USDA NRCS, 2007; Tafur, 1995). The biogas is composed of methane, carbon dioxide, and small amounts of other compounds such as hydrogen sulfide (Rasi et al., 2007). Anaerobic digestion of animal manure has multiple benefits, including renewable energy production, reductions in Greenhouse Gas (GHG) emissions, odor control, and reductions in manure pathogenicity (Yiridoe et al., 2009). Despite these benefits, AD deployment rates are low for US Farms (USDA NRCS, 2007).

Farm-scale AD was first adopted in the US during the oil crisis in the 1970s (USDA, 2008). Despite technological advancements over the past 40 years, a 1998 study reported failure rates approaching 50% in manure-fed AD systems (NREL, 1998). In the past decade, policy changes and developments in AD technology have yielded only mild improvements in deployment rates. Kramer (2004) surveyed 23 digesters from 2002 to 2004, and found that five of the digesters that were operational in 2002 had ceased to operate by 2004. In 2006, AgSTAR reported a doubling in the number of digesters operating in the US between 2004 and 2006 (AgSTAR, 2006). According to data reported by AgSTAR in 2009, however, AD deployment rates are far below 1% based on the number of total animal facilities, and approximately 2% based upon the number of facilities that the US Environmental Protection Agency (EPA) has identified as being suitable for AD (AgSTAR, 2010).

In December, 2009 the US Secretary of Agriculture announced an agreement with US Dairy Producers to reduce GHG emissions from dairy operations by 25% before 2020; anaerobic digestion was cited as the primary method for meeting this goal (USDA, 2009). Such an increase in deployment will require us to understand and to develop methods for overcoming current barriers to AD deployment at dairies.

The University of Florida and the University of California, Davis, both have spreadsheet models available online to evaluate the economic feasibility of AD (Florida Dairy Extension, 2010 and California Biomass Collaborative). However, these models require the user to provide capital and operating costs, meaning that the models are not suitable for production of total costs based simply on operation size. AgSTAR has also developed a model to help farmers determine the economic viability of AD. The model requires several site-specific parameters which are critical to the prediction of costs at one location, but they also mask the larger economic realities of AD. To uncover these realities, a simple model that incorporates fewer site-specific inputs and that provides a first-level approximation accounting for odor and GHG benefits is needed. The goals of our work included creating such a model, which we call the Simplified Framework for Analyzing AD (S-FAAD), validating the model, identifying critical constraints, and making recommendations for improving AD deployment.

Materials and Methods

The S-FAAD model was implemented in Microsoft Excel, with all computations being done using normal cell formulae. Visual basic for applications (VBA) code was written to enable ranges of input variables to be tested, to study the breakdown of costs, and to perform a sensitivity analysis. The S-FAAD model computes a price ($\$/\text{m}^3$) for the biogas

produced from AD, taking into account the capital and operating costs of the digester, as well as crediting cost avoidances due to odor and GHG abatement. By assuming a biogas energy density (GJ/m^3), the cost of energy (as methane) in the biogas ($\$/\text{GJ}$) is computed. This is a crucial value, because it allows us to compare the cost of AD-generated energy to its commercial competitor: natural gas. The comparison to natural gas may appear unfair, since AD brings multiple other benefits and possibilities, including, but not limited to, (1) GHG reductions, (2) odor reductions, and (3) the possibility to use the biogas in engine generators to produce electricity and heat. Regarding the first two issues, S-FAAD provides explicit dollar credits the AD system for GHG reductions, and for odor reductions. The final concern – that the economics of AD are improved if conversion to electricity is achieved – is only valid if renewable-energy tax credits or similar incentives are available. If such credits are not available, then conversion to electricity is unlikely to have any economic benefit, otherwise farms across the US would be purchasing low-cost natural gas and generating their own electricity on-site.

The endpoint of the S-FAAD model is computation of a value we term the methane cost ratio (MCR). The MCR is a dimensionless number, found by dividing the biogas energy cost (in $\$/\text{GJ}$) by the commercial price of natural gas (also expressed in $\$/\text{GJ}$). We posit that MCR is a key indicator of AD deployment: if MCR is above 1.0, commercial energy is cheaper than digestion-derived energy, making digester deployment and long-term operation unlikely. Conversely, if MCR is below 1.0, digester-derived energy is cost-competitive with commercial sources, making long-term operation of digesters more likely. To obtain the MCR, several operating parameters and costs are considered as shown below in figure 1.

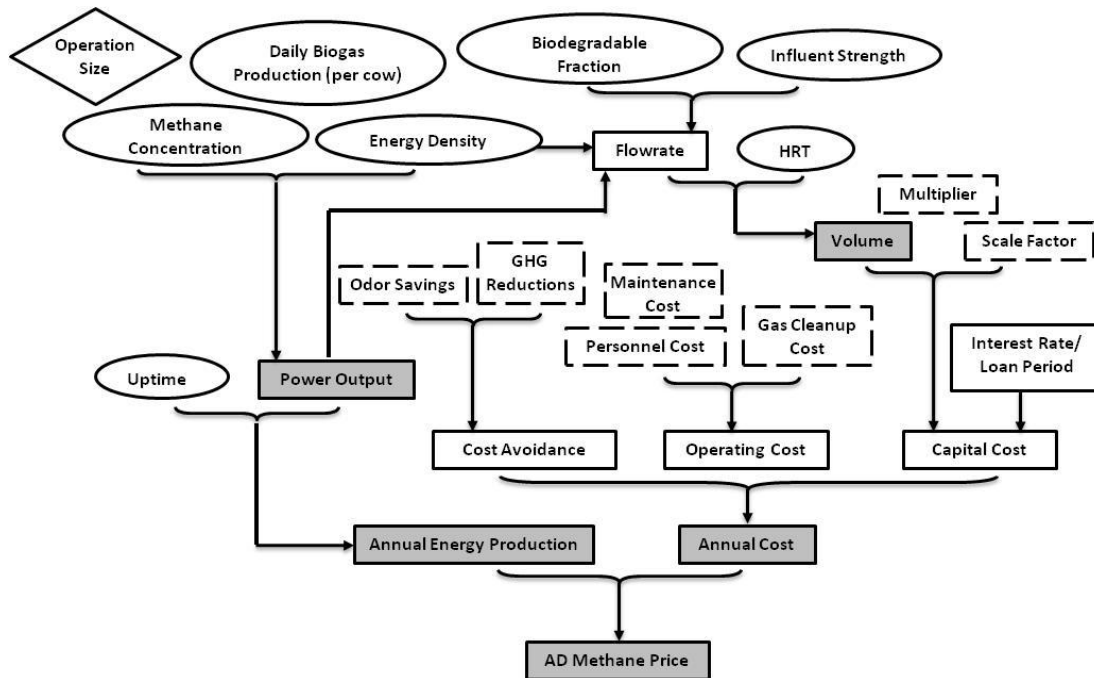


Figure 1. S-FAAD Flow Chart.

Diamonds represent user inputs, ovals represent assumed values, rectangles represent computed values, dotted rectangles represent computed values based on assumptions not shown, and shaded rectangles indicate primary outputs.

Figure 1 summarizes the data flow in S-FAAD. The operation size and assumptions for digester operation and biogas production rates are used to calculate the cost for producing methane via AD. This value is then compared to the market natural gas prices to determine the MCR. The S-FAAD model can be broken down further into operating parameters and annual expenses and revenue sources.

Operating Parameters and Assumptions

The principle assumptions for dairy manure and biogas production include the hydraulic retention time (HRT), influent strength, fraction of manure biodegraded, methane

concentration, daily biogas production per cow, and the energy density of manure solids. The S-FAAD model assumes a 20-d HRT which falls into the typical range for plug-flow digesters (Wilkie, 2005). Influent strength was assumed as 0.11 kg/L (total solids) which is based on a typical range of 0.11-0.14 kg/L for scrape collection systems for plug flow digesters (USDA, 2007). Manure solids were assumed to have the energy density of cellulose: 17 MJ/kg (GCEP, 2005). The fraction biodegraded assumed to be 26% (Martin et al., 2003; Cornell University, 2008), and a biogas production rate of 1.9 m³/cow-day was assumed (USDA, 2007) as was a biogas volumetric methane concentration of 60% (Ghafoori and Flynn, 2007). These key operating assumptions were used to calculate the annual biogas production, the power output based on the methane concentration and energy content of methane, the biodegradable loading requirement for the digester, the volumetric flowrate into the digester, and the required digester volume.

Annual Expenses and Revenue

To determine the economic viability of AD, S-FAAD computes the capital costs, operating costs, carbon tax credits, and odor abatement savings. For all these values, it is assumed that there is enough demand on the farm to use all the biogas produced.

Capital Cost

The capital cost for the digester (C_{GC}) is determined from the digester size using a standard scaling equation (eq. 1) (Brown, 2003):

$$C_{GC} = M \times V_D^{SF} \quad (1)$$

Where SF is a scaling factor and M is a multiplier. Although tabulated values of SF and M are available for many unit operations (e.g., Brown, 2003), we are unaware of such figures

being available for anaerobic digesters. However, AgSTAR (2009) compiled tables containing the grassroots capital costs for plug flow digesters built between 2005 and 2008, and used the data to find the following equation relating the capital cost to operation size (eq. 2):

$$C_{GC} = 617 \times S_{op} \times 566,000 \quad (2)$$

AgSTAR's equation includes the digester cost as well as equipment, installation, and engineering costs. Because S-FAAD assumes that biogas is not used to generate electricity, a 36% correction (reduction) was applied based on data presented in USDA (2008). Costs were corrected to 2010 USD, and a power equation was fit to the resulting data across operation sizes from 500 to 3000 (AgSTAR, 2009). The resulting scale factor and multiplier were 0.59 and \$13,575 (\$/cow) respectively, with $r^2=1$. It is interesting to note that plug-flow digester costs appear to follow a "six-tenths" rule as is often seen in process equipment (Brown, 2003).

Operating Costs

The operating costs considered in S-FAAD include personnel costs and gas cleanup costs. Peters et al. (2003) provides typical labor requirements for continuous flow reactors. Using this value, the labor requirement is approximately 4 hours/day, or 50% of a full-time employee (FTE). The annual cost for one FTE is assumed to be \$40,000. As the size of the digester and pumps increase, the operator time required is not expected to change significantly; thus in S-FAAD labor requirement is treated as independent of digester size.

There are several levels of biogas cleaning, with the simplest typically involving moisture and hydrogen sulfide removal, and sophisticated cases removing carbon dioxide to create

pipeline quality natural gas. Gas cleanup costs that range from \$0.03-\$0.14 per cubic meter biogas are cited by USDA (2007) based on updated costs from Walsh et al. (1988). A gas cleanup cost of \$0.03 per cubic meter biogas was used for the baseline calculations, but the impact of higher gas cleanup costs was also explored.

Maintenance Costs

The maintenance cost was calculated based on the reactor cost. According to Peters et al. (2003) maintenance costs run between 2%-11% of the fixed-capital investment cost each year depending on the process. Based on this a value of 5% was selected.

Carbon Credit Savings

Anaerobic digestion reduces GHG emissions in two ways: by reducing direct GHG emissions from a non-AD waste management method, and by avoiding fossil carbon burning through the use of digestion-generated methane instead of natural gas. US EPA (2009) was used to calculate GHG emissions reductions for using AD instead of a liquid slurry storage structure. The emissions offset by using AD methane instead of natural gas were then calculated from the CO₂ emissions resulting from combustion. Note however that GHG emissions associated with digester construction as well as other indirect emissions were ignored in this analysis. To convert these GHG reductions into economic values, a carbon-credit approach was used. Metcalf (2009) suggests that carbon credits in the US be valued at \$15-\$20/ton CO₂. Therefore, a value of \$20/ton CO₂ equivalent was used as a baseline value in S-FAAD.

Odor Abatement Savings

To put an economic value on the odor reductions cause by AD, we credited the AD operation with the net increase in property values that would occur due to a reduction in odor emission. This required an estimate of the area (acres of property) adversely affected by odor prior to AD installation, and an estimate of the property devaluation that occurs due to odors. Odor set-back distances (PAAQL, 2006) were used to determine the impact area, and data from a hedonic study was used to estimate reductions in property values (Herriges et al., 2005). The Herriges et al. (2005) work evaluated the impact of hog operations on property values in five counties in Iowa using a hedonic price model. No similar data was found for dairy manure odors; therefore, S-FAAD uses property devaluations based on the hog operation study. Reductions in property values varied with facility size, distance, and wind direction, but averaged 2% (Herriges et al., 2005). The set-back distance used was based on guidelines developed by Purdue University's Agricultural Air Laboratory (PAAQL, 2006). A simplified equation was obtained from average values assumed in the PAAQL model (*equation 3*) where the offset distance (D) is in miles and S_{op} is the operation size (number of cows).

$$D \cong 4.4E - 4 \times S_{op} \quad (3)$$

This equation assumes that no odor abatement technology is used. When AD is utilized for odor abatement, the impact distance is reduced by applying a correction factor of 0.88 (PAAQL, 2006). We assumed a property rental rate of \$14,000/ha/yr, and computed a cost benefit for AD based on a reduction in impacted area.

The odor reduction estimates do not capture non-manure odor emissions on the farm and therefore, our cost estimates may be overly optimistic. Furthermore, although the economic benefits associated with odor reduction may be real, there are currently no mechanisms for these benefits to accrue to the digester operator, so their inclusion here is highly favorable toward AD. It was important to include this term to put an economic perspective on a commonly-claimed AD benefit (Wilkie, 2005).

Sensitivity Analysis

To understand how the assumed values impacted the calculated MCR, a sensitivity analysis was completed. Sensitivity coefficients – that is, percent changes in output per percent change in inputs – were computed about the baseline value (Hamby, 1994).

Results and Discussion

Model Validation

To validate the model, FarmWare 3.4 was used as the standard, and a baseline scenario was developed to compare S-FAAD to FarmWare 3.4. Simulations in FarmWare 3.4 assumed that the dairy farm is located in Iowa, cattle are confined in a freestall scraped barn, the method prior to AD used for manure management is a storage tank containing manure and milking center wastewater, and propane is the replacement fuel (natural gas not available). Data points were collected for 200, 400, 600, 800, and 1000 cow operations, with all costs in 2010 USD (Figure 2).

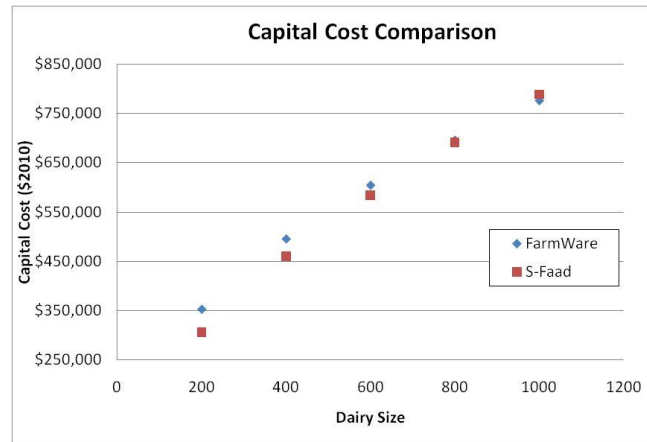


Figure 2. Capital Cost Comparison.

As showed in figure 2, the capital costs reported by FarmWare 3.4 and S-FAAD are very similar. For dairy farms with more than 600 cows, the capital cost reported by S-FAAD is almost the same (within 3%) as the value reported by FarmWare 3.4. For farms with 200 or 400 cows, the percent difference between S-FAAD and FarmWare 3.4 increases slightly. Based on the operation size ranges discussed in AgSTAR (2009) which range from 500-3000 dairy cows, it is reasonable that the difference in the values reported by FarmWare 3.4 and S-FAAD would increase outside of the range originally surveyed by AgSTAR. Despite these differences for smaller farm sizes, figure 2 demonstrates that S-FAAD provides an accurate first-order estimate for the capital cost of AD using fewer site-specific parameters and inputs.

Baseline Results

Using the baseline assumptions of 7% interest rate, 20 yr amortization period, 90% uptime, \$20/Mg carbon value, and \$0.03/m³ gas cleanup cost, and a natural gas energy cost of \$5.29/GJ (based on a 2010 average), MCRs ranged from 1.4 for the 1000-head facility, to nearly 4.1 for the 200-head facility. The 1.4 value suggests that energy from anaerobic digestion would cost 140% of pipeline natural gas, making anaerobic digestion not

economically viable. Breakeven (i.e., MCR of 1.0) occurs around 1700 head under the baseline assumptions, which appears to be a reasonable value since the median herd-size at dairies using AD is 1300 (AgSTAR 2010).

Impact of Interest Rate, Amortization Period, Uptime, Carbon Value, and Gas Cleanup

Costs on MCR

The MCR was highly sensitive to interest rates, as shown in figure 3. Anaerobic Digestion becomes economically viable for farm sizes greater than 1000 as the interest rate approaches 1%, but interest rates alone are not sufficient for an 800-cow dairy to become economically feasible.

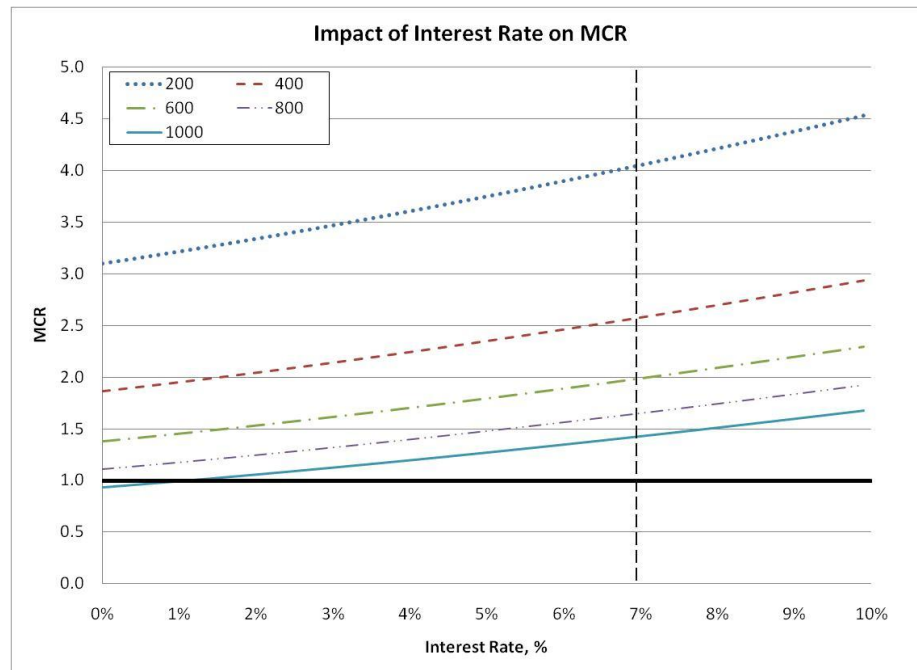


Figure 3. Impact of Interest Rate on MCR.

The dotted line illustrates the baseline value for interest rate and the solid black line illustrates the break-even point.

Amortization period – which in S-FAAD is a surrogate for system life expectancy – is also a key driver of MCR, as shown in figures 4. While the amortization period alone doesn't provide an economically viable solution for any of the sizes evaluated, it is important to note that as the amortization period decreases, the MCR goes up significantly. This simply drives home the importance of well-designed and long-lived systems on overall process economics.

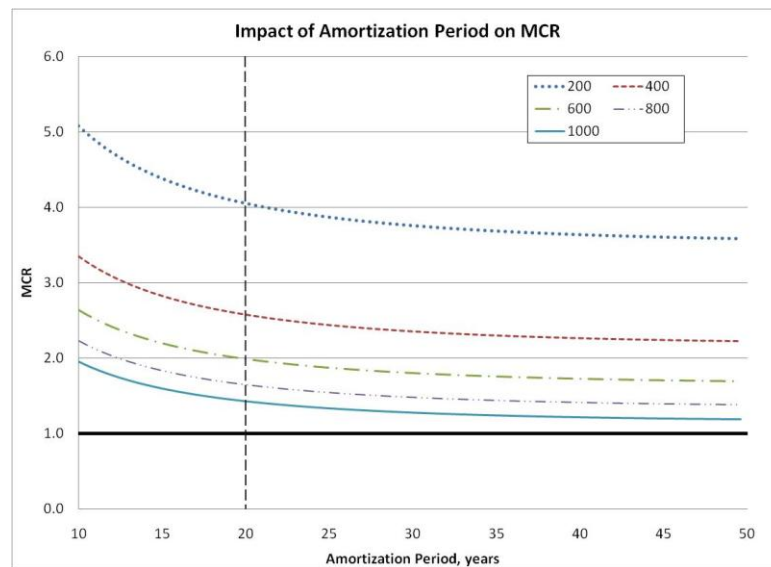


Figure 4. Impact of Amortization period on MCR.

The dotted line illustrates the baseline value for the amortization period and the solid black line illustrates the break-even point.

Well-designed systems should not only last a long time, they should be operational for a large fraction of the year. Figure 5 illustrates the enormous impact of uptime on the economic viability of AD systems. A 30% drop in the MCR results in a 50% increase in the MCR for operation sizes of 200. Multiple challenges to high uptime have been cited by farms running digesters, including equipment reliability, foam and crust formation in the digester, and proper temperature control (Cornell University, 2008).

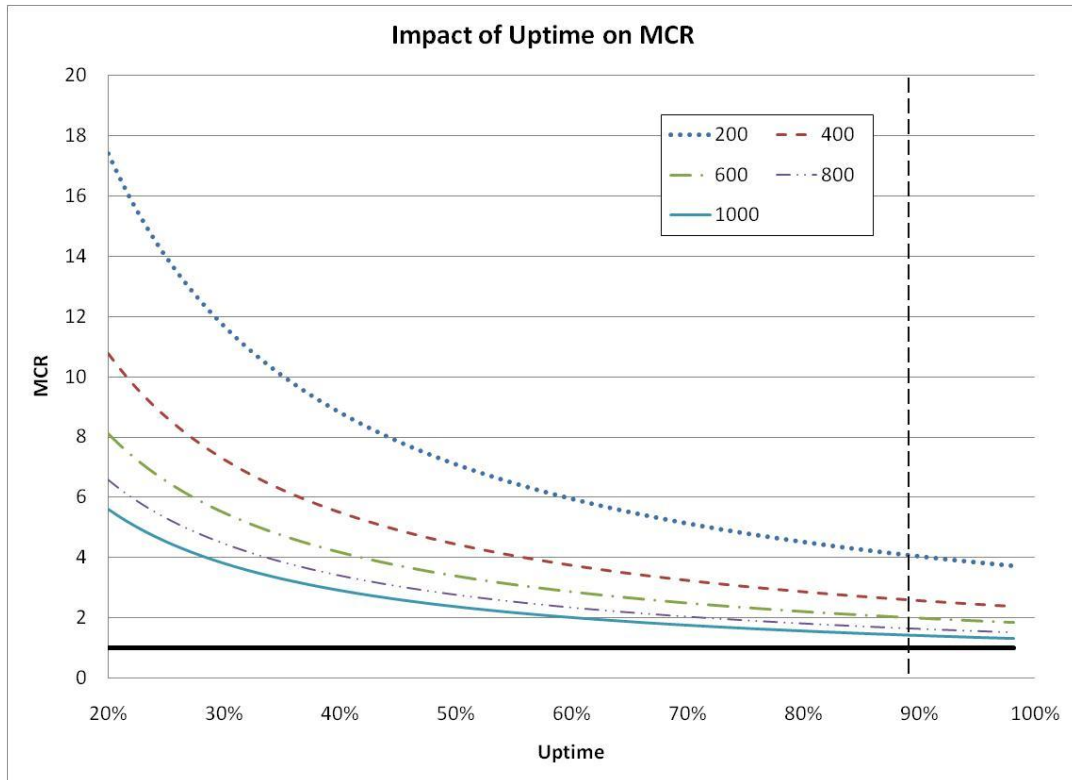


Figure 5. Impact of Uptime on MCR.

The dotted line illustrates the baseline value for the uptime and the solid black line illustrates the break-even point.

The base-case used a literature-suggested value for carbon credits in the US of \$20/metric ton CO₂ (Metcalf, 2009). However, CO₂ market prices haven't exceeded \$3.50/metric ton on the Chicago Climate Exchange (2010). Figure 6 shows how important carbon-values are to viable AD, in light of the relatively low commercial energy prices in the US. With carbon values near actual market values, and with all other inputs at base case levels, none of the scenarios tested is economically viable. The best case system is the 1000-head system, with an MCR around 1.4.

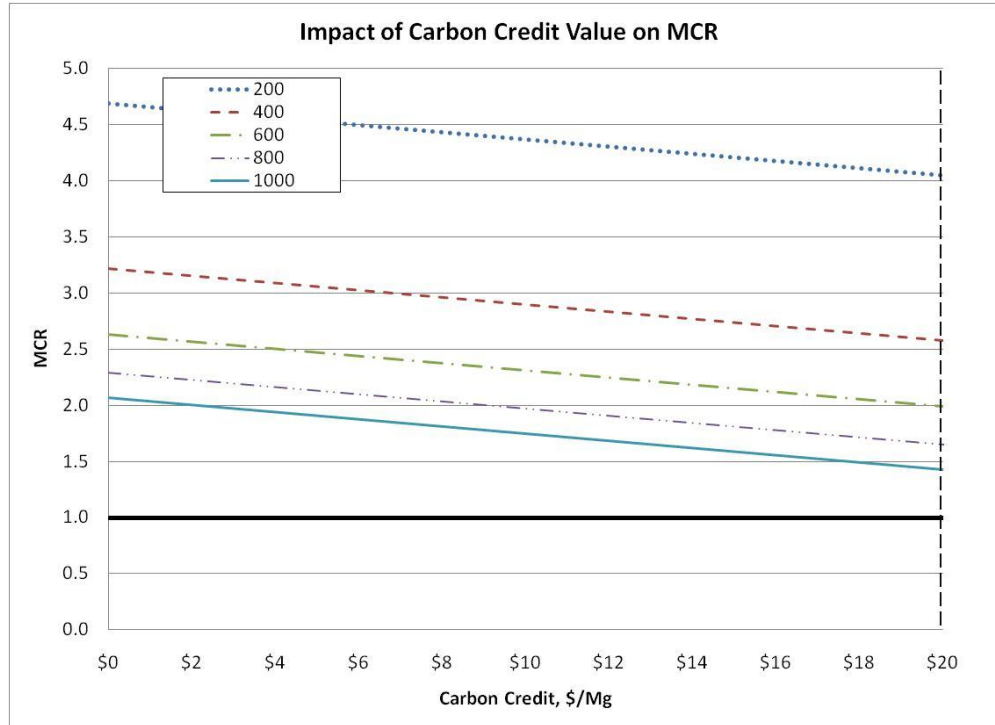


Figure 6. Impact of CO₂ Value on MCR.

The dotted line illustrates the baseline value for the CO₂ credit and the solid black line illustrates the break-even point.

As discussed in previous sections, the gas cleanup costs vary significantly based on the type of conditioning required. As shown in figure 7, if gas cleanup only involves hydrogen sulfide removal (\$0.03/m³ biogas), then 1000 cow dairies are close to being economically viable; however, as the gas cleanup cost increases, so does the MCR.

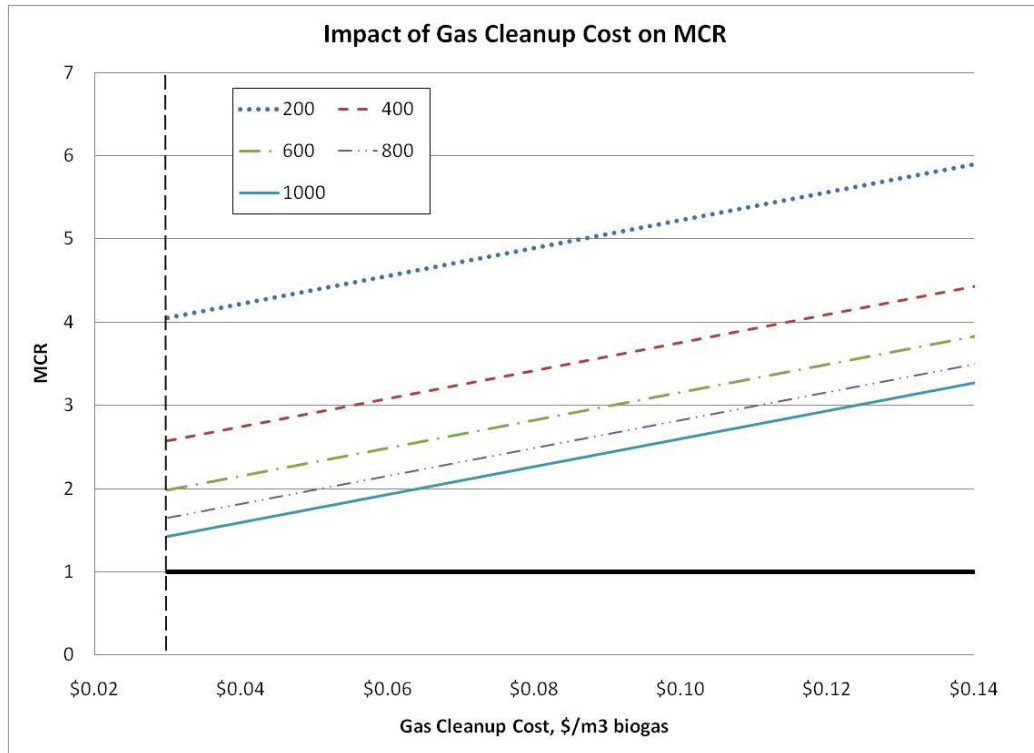


Figure 7. Impact of gas cleanup cost on MCR.

The dotted line illustrates the baseline value for gas cleanup costs and the solid black line illustrates the break-even point

Cost Breakdown

To better understand the annual cost for installing and operating a digester, the percent of the total cash flow represented by each expense and cost benefit was determined. Figure 8 illustrates how costs breakdown over the range of operations studied.

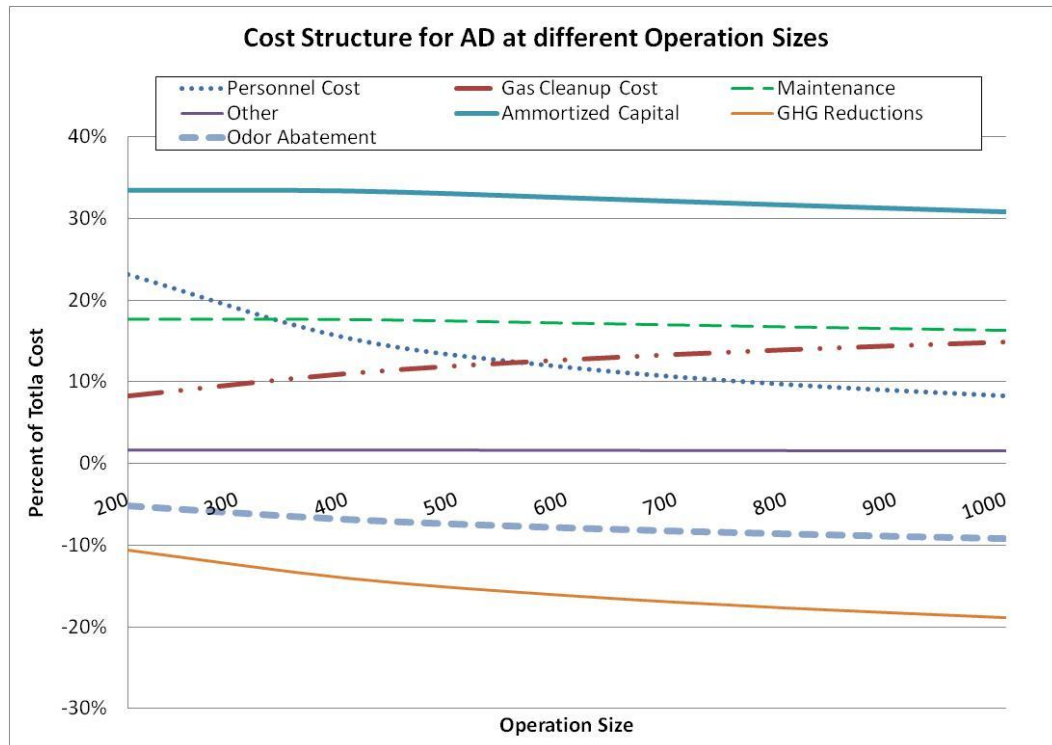


Figure 8. Cost Breakdown vs. Operation Size.

Revenue streams are shown on the graph as negative percentages and annual costs are shown as positive percentages.

Figure 8 shows that amortized capital costs dominate the overall cost of AD. As the operation size increases, this term drops slightly, but still remains above 30% for 1000-cow dairies. Based on these results, decreasing amortized capital costs appears to be the most effective way to improve AD deployment rates and decrease the MCR. Decreases in amortized capital costs can be realized in a multitude of ways, including: (1) improved structural design to reduce actual digester construction costs without sacrificing longevity and reliability, (2) improved structural design to increase expected lifetime and thereby lengthen amortization period, (3) provision of low-cost loans or matching funds for digester construction, or (4) improved bioprocess engineering to enable equal degradation at lower

retention times (thus decreasing reactor size and cost while maintaining gas production). It is important to emphasize that it is *amortized capital cost*, and not simply *capital cost* that must be decreased: digesters made using low-cost materials such as tubular polyethylene bags (Lansing et al., 2008) may require replacement after a few years and can only be compared to other systems on an amortized capital cost basis.

These graphs assume a gas cleanup cost of $\$0.03/\text{m}^3$ biogas. If CO_2 is removed from the biogas at $\$0.14/\text{m}^3$ the gas cleanup cost overtakes capital cost for all operation sizes.

Another important variable to note is the natural gas price. Natural gas prices fluctuate significantly. In S-FAAD, the natural gas price is the denominator in the MCR and is directly tied to AD economics. If natural gas prices increase to the peak prices realized in 2008, the outlook for AD becomes much brighter; however, as long as natural gas prices remain low, AD struggles to be an economically viable solution, especially on smaller dairies.

Sensitivity Results

The terms with the highest sensitivity coefficients are shown in Figure 9. Sensitivity coefficients indicate the percent change in MCR resulting from a 1% increase in the variable listed: For example, a 1% increase in the operation size from the base case causes a -0.6% drop in MCR. The scale factor used in equation 1 had the greatest sensitivity coefficient, as expected. While this value cannot be readily adjusted to improve AD economics, its high sensitivity coefficient illustrates the importance of accurately estimating this term. The multiplier is the second most sensitive variable. Unlike the scale factor, this value could be changed via technological advancements improving AD digester design. The uptime for a

digester heavily impacts AD economics as shown below; we believe many operational AD's struggle with this. Unsurprisingly, the market natural gas price is also highly sensitive and market fluctuations in natural gas price can drastically change the economic outlook for AD.

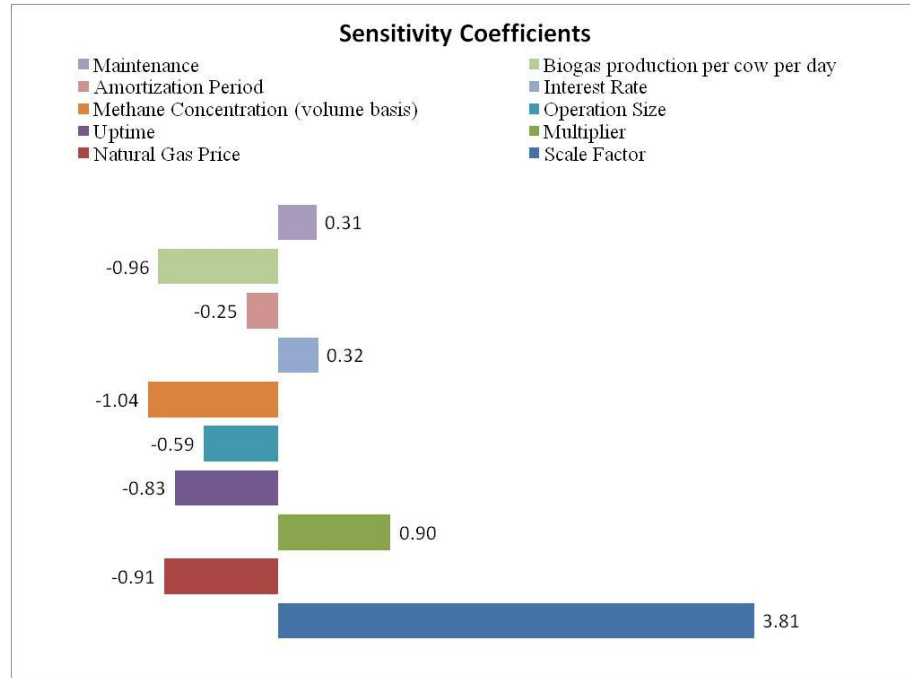


Figure 9. Sensitivity Analysis Results.

Conclusions

The Simplified Framework for Analyzing Anaerobic Digestion (S-FAAD) reported here showed that digester capital costs dominate the overall cost of producing energy using anaerobic digestion. Using the \$20/Mg carbon prices that have been suggested in the literature, achieving the US Secretary of Agriculture's GHG emissions reduction goals is feasible if the natural gas price is high. In reality, CO₂ values are not as high as predicted and

gas cleanup costs may not be as low as predicted. Under these more realistic assumptions, S-FAAD showed that the low commercial energy prices in the US mean that without price supports (in the form of carbon credits, or low interest loans, or grants), even at 1000 animal herd sizes, biogas from AD cannot compete with pipeline natural gas. Therefore, evaluating policy changes and technological advancements that could lead to increases in digester life and decreases in amortized digester cost and interest rates is recommended.

Acknowledgements

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CHAPTER 3. FERMENTATION MODELING: KINETICS AND THE BOTTOM LINE

A paper to be submitted to *Biotechnology and Bioengineering*

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Abstract

Advances in metabolic engineering enable increasing production of biorenewable chemicals and economic evaluations can provide insight into impacts of different kinetic parameters on the cost structure of fermentation. The Fermentation Economic Modeling Tool (FEMT) was developed to evaluate these critical factors with the primary output being an order-of-magnitude estimate for the product production cost. Results showed that three key kinetic and operating parameters – fraction of the product in the biomass, substrate concentration, and yield—have the greatest impact on the production cost. These results demonstrate the utility of simple models to provide insight into how fundamental bio-kinetic parameters influence production costs.

Introduction

Tremendous technological growth and advancement took place during the industrial revolution resulting in an increased demand for petroleum-based products, including energy, transportation fuels, and chemicals. Biochemical routes, previously used to produce chemicals, could no longer compete with their low-cost, fossil-based counterparts and these technologies faded away (Engel et al., 2008).

As the world population continues to rise, fossil-based resources are depleting more rapidly than they can be regenerated (Rojan et al., 2007). This realization has led scientists to reconsider biochemical production routes, namely industrial fermentation (Rojan et al., 2007). New fields such as metabolic engineering have enhanced our understanding of fermentation processes and the microbial mechanisms that control these processes. This has led to new microbial strains with improved kinetic properties; however, improvements to microbial metabolism often involves tradeoffs (Huang and Tang, 2007), i.e., a 10% increase in substrate concentration may result in a 10% decrease in the maximum specific growth rate for an organism. The impact of kinetics and tradeoffs between kinetic variables on process economics is not well-documented. For industrial processes, kinetic parameters are considered proprietary and are not published (Sauer et al., 2007). Lab and pilot-scale studies for several chemicals are widely published and available; however, very few of these studies quantify process economics. Several studies use the term “economics” loosely and state that a process is or is not economically feasible without providing detailed analysis or justifying this conclusion (e.g., Engel et al., 2008, Rojan et al., 2007, Stahmann et al., 2000, Li et al., 2001). Numerous metabolic engineering papers describing improved microbial strains do not discuss process economics at all (Bellissimi and Ingledew, 2005, Kim et al., 2007). While

economic evaluations are often outside of the scope of a metabolic engineering effort, understanding which variables have the highest impact on the process economics and having a general understanding of these impacts during the metabolic engineering phase of research could lead to more directed research efforts and improve the likelihood of industrial deployment.

Studies that do incorporate process economics were also evaluated (e.g. Choi and Lee, 1997; Tao and Aden, 2009; Akerberg and Zacchi, 2000; Qureshi and Blaschek, 2000); however, some of these models did not provide a breakdown of the production costs and others were too complex and required site and process-specific parameters limiting general use for multiple processes. While models derived from programs like ASPEN provide detailed analysis for a specific process, they cannot be used to evaluate trends in cost over ranges of different variables and sizes for a variety of operations without extensive knowledge of different processes.

The goal of this work was to develop a relatively simple tool that allows insight into the key tradeoffs and cost trends between different fermentation variables. While this model is not suitable for specific site cost prediction, it provides first-level approximations that can be used by metabolic engineers to develop more efficient bacterial strains.

Materials and Methods

The FEMT (Fermentation Economic Modeling Tool) was implemented in Microsoft Excel, with all computations being done using visual basic for applications (VBA) code. The FEMT utilizes a kinetic model that is integrated with economic calculations to function as a

simple dynamic model for first order approximation of the unit operation processing cost in terms of 2010 USD per kg product. Figure 1 illustrates the inputs and outputs for the FEMT.

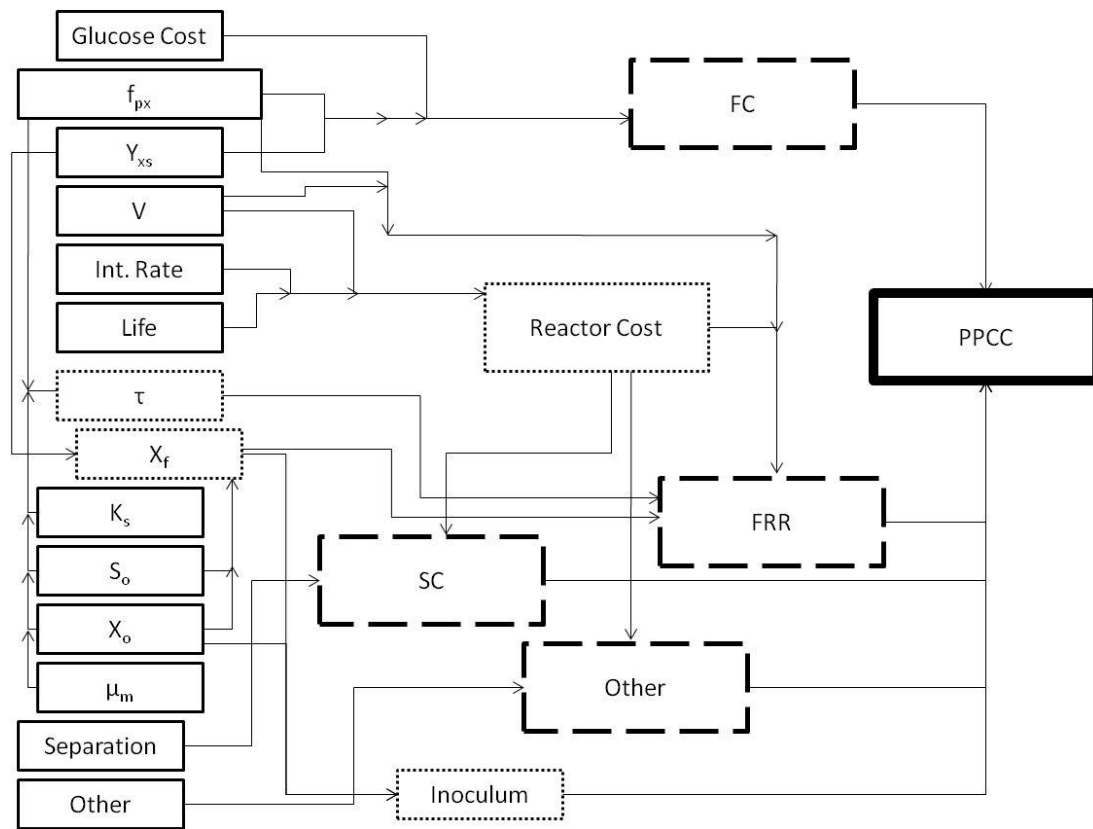


Figure 1. FEMT Flow Diagram. All inputs for the model are outlined in a thin solid line, all intermediate calculations in a thin dotted line, primary outputs are shown in a thick dotted line, and the product production cost is shown in a thick solid block.

The primary feedstock for the model is assumed to be glucose; however, the model could be adapted to other feedstocks. Glucose undergoes fermentation to produce a designated chemical or intermediate product of interest. The calculated cost for this fermentation product incorporates the feedstock cost, reactor rental rate, separation cost, and a first level approximation of energy and labor cost as shown:

$$PPCC = \frac{(FC+FRR+SC+OC)}{1-inoc} \quad (1)$$

As shown in equation 1, the product production cost is the sum of the feedstock cost (FC \$/kg product), fermentation rental rate (FRR, \$/kg product), separation cost (SC, \$/kg product), and other cost (OC, \$/kg product). This total is then corrected to account for the percent inoculum (inoc) required in the reactor to determine the corrected product production cost (PPCC, \$/kg product). Each variable in equation 1 is described in further detail below.

Feedstock Cost

The feedstock cost for glucose is an input for the FEMT; however, the units are 2010 USD per kg feedstock while PPCC is in 2010 USD per kg product. To account for this, the glucose cost (GC, \$/kg glucose) is converted to 2010 USD per kg product using the fraction of product in the biomass (f_{px} , %) and the product yield (Y_{xs} , kg biomass/kg glucose) as shown in equation 2.

$$FC = \frac{GC}{f_{px} \times Y_{xs}} \quad (2)$$

Fermentation Rental Rate

The FRR is the amortized capital cost for the reactor (RC, \$) divided by the annual production capacity (AP, kg product). Calculation of the fermentation rental rate (FRR) requires knowledge of the kinetic limitations of the microorganism used for fermentation and the process economics for computing the amortized capital cost. Each of these calculations is outlined below.

Annual Production capacity

To calculate the annual production capacity, the retention time, or time required for fermentation must be calculated.

Using a combination of the Monod equation, growth equation, and an equation for the yield of cell mass from substrate concentration as described for batch reactors by Shuler and Kargi (2002), the Logistic equation is formed as shown in eq. 3.

$$\mu_m t = \frac{K_S Y_{x/s} + S_0 Y_{x/s} + X_0}{Y_{x/s} S_0 + X_0} \ln \frac{X_f}{X_0} - \frac{K_S Y_{x/s}}{Y_{x/s} S_0 + X_0} \ln \frac{Y_{x/s} S_0 + X_0 - X_f}{Y_{x/s} S_0} \quad (3)$$

In this equation, we assume that the final titer, X_f (g/L), is equal to 95% of the maximum theoretical value given in Shuler and Kargi (2002), $Y_{x/s} S_0 + X_0$. This expression can then be used to calculate the fermentation retention time, τ (hrs). The fermentation retention time is then corrected to account for downtime between loading and this corrected value is used in additional calculations relating to the production cost. Additionally, the inoculum requirement can be calculated by dividing the initial titer, X_0 (g/L) by the final titer, X_f (g/L).

The annual production capacity can then be calculated as shown below.

$$AP = \frac{X_f \times f_{px} \times V}{\tau} \quad (4)$$

As shown in equation 3 the final titer (X_f kg product/m³) is multiplied by the fraction of product in the biomass (f_{px} , %) and reactor volume (V , m³) and then divided by the retention time (τ , converted to yr).

Annual Capital Cost

The annual capital cost accounts for the grassroots capital cost for installing the reactor as well and the interest rate and reactor life. The grassroots capital cost is computed using standard scale factors and multipliers as discussed in Brown (2003) and takes into account engineering, labor, materials, freight, and construction costs associated with a piece of equipment. The fermentation vessel is assumed to be a vertical process vessel with a unit cost of \$7300/m³ (USD 2010), a scale factor of 0.71, a materials module factor of 1.04, and a labor module factor of 0.49. The amortized capital cost is then calculated based on a user-specified reactor life and interest rate.

Separation Costs

Separation costs vary significantly from one operation to another and without additional processing data, it is difficult to predict the separation cost. Therefore, the separation cost used in FEMT is given as a percentage relative to the annual reactor cost.

Other Costs

Due to regional and processing differences in labor, electricity, cooling water, and natural gas prices, these variables were not considered specifically within the model; however, an “Other” category was incorporated into the model as a first approximation for these variables. This category, like the separation cost, is also given as a percentage relative to the annual reactor cost.

Sensitivity Analysis

To understand how the assumed values impacted the calculated PPCC, a sensitivity analysis was completed. Sensitivity coefficients, or the percent changes in output per percent change in the inputs, were computed (Hamby, 1994).

Results and Discussion

The FEMT is designed for metabolic engineers to use in evaluating a specific process; however, to review a single process, all of the kinetic and operating parameters used in the model should ideally come from a single source. A review of literature on batch fermentation processes for biorenewable chemical production was completed and no single sources were found containing all the necessary inputs. These findings illustrate the need for continuity and a reporting methodology in papers concerning microbial fermentation. While some papers reported the fermentation time and productivity, others reported the initial and final substrate concentration and the yield (Demain, 2009, Wingren et al., 2005, Altinas et al., 2002, Nakamura et al., 1996, Bai et al., 2008). One article discussed kinetic and economic results but never gave the reactor volume (Akerberg and Zacchi, 2000). Another article reported all of the necessary data, but it appeared that there was an error in one or more of the kinetic parameters reported (Heinzle et al., 2006). Without a clear and concise reporting system for kinetic data, comparisons between different papers and microbial strains cannot be made.

Because limited data was available in the literature for different fermentation processes, ranges of data were evaluated rather than individual values for a specific process.

Four variables were investigated initially, including the fraction of the product in the biomass (f_{px}), maximum specific growth rate (μ_{max}), initial substrate concentration (S_o), and separation cost. An optimistic and pessimistic value was selected for each parameter and all combinations were evaluated as shown in Table 1.

Table 1. Simulation Test Cases.

	f_{px} (kg product/ kg biomass)	S_o (g glucose/ L broth)	μ_m (hr ⁻¹)	Separation Cost
Case 1	2.7	100	1.5	200%
Case 2	2.7	100	1.5	500%
Case 3	2.7	100	0.1	200%
Case 4	2.7	100	0.1	500%
Case 5	2.7	10	1.5	200%
Case 6	2.7	10	1.5	500%
Case 7	2.7	10	0.1	200%
Case 8	2.7	10	0.1	500%
Case 9	0.8	100	1.5	200%
Case 10	0.8	100	1.5	500%
Case 11	0.8	100	0.1	200%
Case 12	0.8	100	0.1	500%
Case 13	0.8	10	1.5	200%
Case 14	0.8	10	1.5	500%
Case 15	0.8	10	0.1	200%
Case 16	0.8	10	0.1	500%

Several different values for these variables are reported in literature, so most of the values shown are for ethanol production using *Saccharomyces cerevisiae*. Altintas et al. (2002) reported an f_{px} value of 2.7 for one of their batch experiment runs. In some cases, an f_{px} value above one would not be reasonable, so a range of 0.8-2.7 was selected. Junker (2004) reported a general glucose substrate concentration of 10-100 g/L and a μ_m range of 0.2 to 0.5 hr⁻¹ for yeast; however, several new fermentations being studied involve bacteria

which have a range of 0.9-2.1 hr⁻¹ and researchers have reported values as low as 0.1 hr⁻¹; therefore, a range of 0.1-1.5 hr⁻¹ was selected. Akerberg and Zacchi (2000) evaluated the cost breakdown of lactic acid produced via fermentation from wheat flour. Their model predicted that the separations capital cost would be twice that of fermentation and that separations and recovery combined would be five times as great. Therefore, a range of 200-500% was selected.

Other inputs for the model remained constant throughout the simulations. Table 2 show the values used for each remaining variable.

Table 2. Base-case Variables.

Variable	Value	Reference
Y _{xs} (dimensionless)	0.115	Altintas et al. (2002)
Fermenter Volume, V (m ³)	1500	
Interest Rate	15%	Keeling personal communication (2011)
Reactor Life (years)	15	Rowe and Margaritis (2004)
Downtime between runs (hrs)	10	Christiansen personal communication (2011)
K _s (kg/m ³)	1	Erickson and Stephanopoulos (1986) and Arellano-Plaza et al. (2007)
X _o (kg/m ³)	1	Richard and Margaritis (2004)
Other	80%	Tao and Aden (2009)

Results were determined as ranges for each scenario based on the glucose cost as shown in figure 2. For example, Scenarios one and two illustrate the predicted processing

cost based on optimistic values of f_{px} , S_0 , μ_m , and separation cost over the range of potential glucose prices.

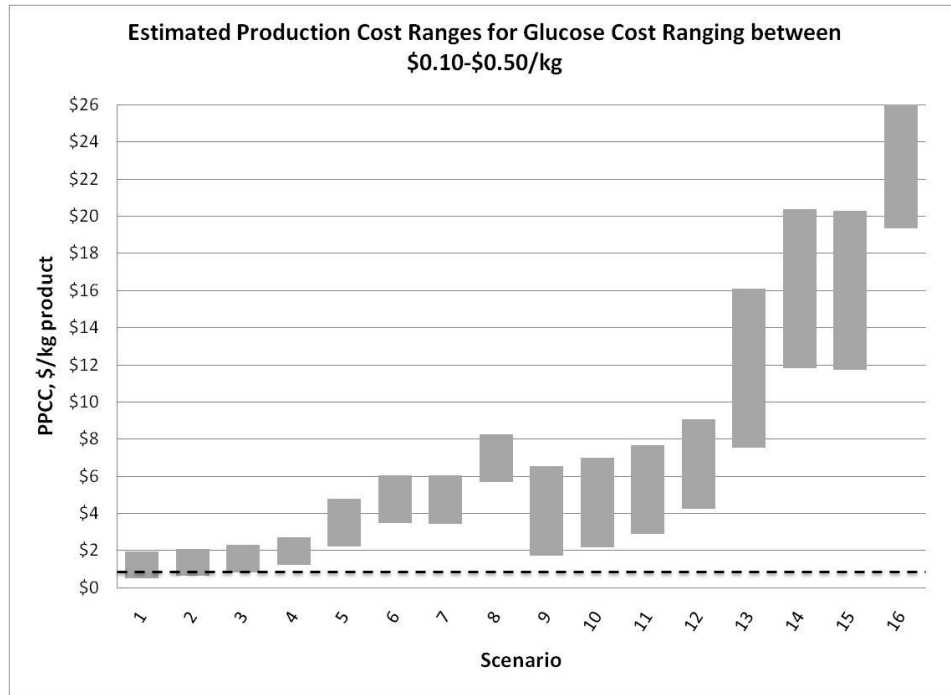


Figure 2. Impact of Glucose Cost on PPCC. The dotted line represents the approximate cost of commodity chemicals.

As shown in Figure 2, the most optimistic conditions are required for the production cost to fall in the commodity chemical range. There are, however, some weaknesses in the model that need to be addressed to make a full comparison between commodity chemical prices and the production cost output by the FEMT. The Monod-based kinetic model used in the FEMT does not account for substrate and product inhibition, a major factor in many industrial-scale fermentations. Because of this, the fermentation times ranged from 0.6 hours to 25 hours. This may be a reasonable estimate for some processes; however, simulations were completed based on values for ethanol which typically have longer fermentation times

(Okafor, 2007). Additionally, the productivities ranged from 8-48 which is significantly higher than productivity ranges reported in literature (Jarboe et al., 2010). Because of this, the annual production rate was inaccurate when compared to industrial scenarios, impacting the product cost reported by the FEMT. Because of this, some of the ranges shown above may be pessimistic and some may be optimistic.

The FEMT can also be used to evaluate the cost structures for different operations.

Figure 3 illustrates how the cost structure changes at different scales.

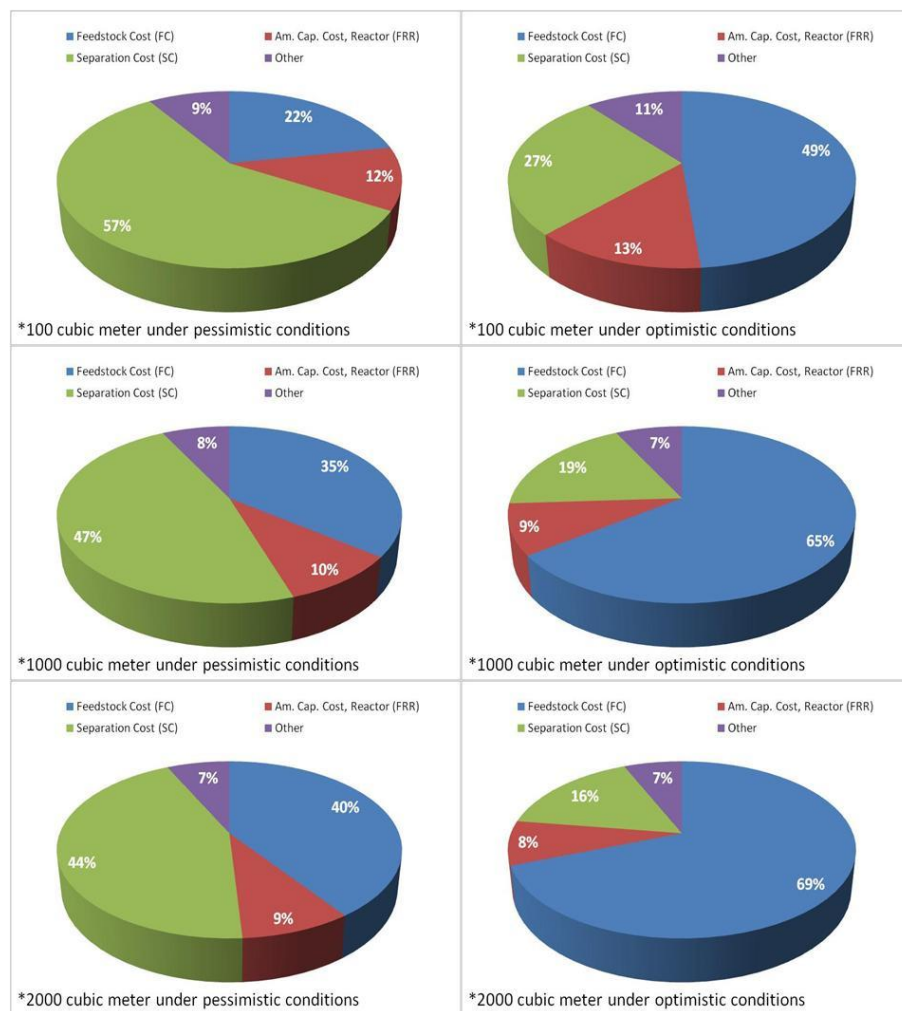


Figure 3. Cost Breakdown for different operation sizes.

As shown in figure 3, the cost breakdown varies greatly between the optimistic and pessimistic conditions. Under optimistic conditions, the glucose cost dominates the product cost in all scenarios; however, when the operating conditions worsen, the separation cost makes up the largest portion of the produced product cost. This is due to the production capacity. As the maximum specific growth rate, substrate concentration, and fraction of the product in the biomass decrease, the annual production does as well, leading to an increase in the fermentation rental cost (\$/kg product) and therefore an increase in the separation cost. One variable not accounted for in the FEMT is the final product concentration. As the product concentration in the broth decreases, the separations cost will increase further. While the separation cost ranges selected illustrate this change to some degree, this portion of the model is not dynamic, so the user needs to adjust the separation percentage based on their knowledge of the product concentration.

A sensitivity analysis was also completed as described in the materials and methods section. Figure 4 illustrates the sensitivity coefficient ranges for each variable based on the simulations described above.

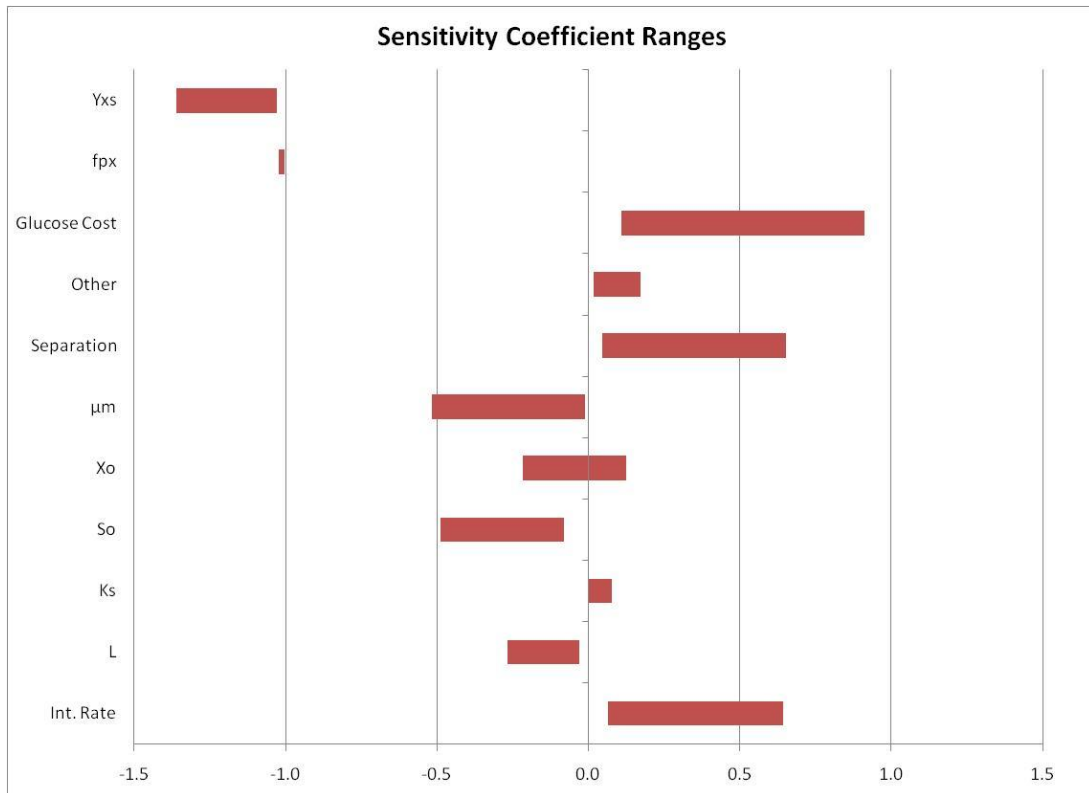


Figure 4. Sensitivity Coefficients.

The sensitivity coefficients shown in figure 4 are illustrated based on their impact they have on PPCC. For example, Y_{xs} and f_{px} have a significant impact on PPCC and as they increase, PPCC decreases. The f_{px} value displayed did not change under the different conditions that were evaluated and is therefore represented with a thin line; however, other terms like the glucose cost varied significantly based on the value used for the glucose cost and the operating parameters. In addition, the initial substrate concentration also significantly impacts the PPCC as expected based on the results described in figure 2.

One thing to note in Figure 4 is the impact of X_o on PPCC. Based on the fermentation conditions there is an optimum value for X_o . X_o remained constant over the

range of values evaluated; however, in some cases, it fell below the optimum value and in other cases was above the optimum value, impacting the PPCC positively or negatively.

Future Work

The results of this research illustrate the importance of yield and the fraction of the product in the biomass on the final production cost for a chemical of interest.

While FEMT provides reasonable cost estimations under optimistic conditions, additional research is needed to adjust the kinetic portion of the model so that it is more representative of realistic fermentations. Many industrial fermentation operations are also simultaneous saccharification and fermentation operations or are fed-batch, allowing for more control over the glucose concentration in the broth and higher final product concentrations and productivities. Looking into methods for allowing the user to select the type of fermentation method is also recommended so that the FEMT can more easily be adapted for different operations.

In addition, work is needed to compare FEMT to existing software programs like ASPEN to quantify the differences seen in the results. Understanding the true impact of scale-up on kinetic parameters and costs by completing a survey of industry would also greatly enhance the techno-economic and metabolic engineering research. The USDA completed a study of ethanol plants in 2002 to quantify the operating, capital, and labor costs for producing ethanol in the US (USDA, 2005). This study didn't reveal any company information or proprietary process data. A similar survey of biorenewable chemical companies would provide a link between research in academia and industrial operation to

help scientists develop targeted research projects leading to improved technology deployment.

Acknowledgements

The authors would like to thank Dr. Jackie Shanks, Dr. Peter Keeling, Dr. Robert Anex, and GPC for their help in model development.

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CHAPTER 4. GENERAL CONCLUSIONS

Fermentation processes can be used to produce chemicals and energy from bio-based renewable resources and reduce dependence on fossil-fuel resources; however, cost remains a barrier to implementing many of these processes. In Chapter 2, anaerobic digestion (AD) was discussed and a framework for modeling the cost structure of AD for different operation sizes was presented. This model, S-FAAD, illustrated the importance of operation size on the cost of AD-produced methane. To reach higher deployment rates of AD, we hypothesized that the cost of AD-produced methane needs to compete with market natural gas prices. For larger operations, above 1000 dairy cows, this can be realized assuming \$20/metric ton CO₂ trade rates and lower interest rates based on our analysis; however, for smaller operations to succeed, more extreme changes in the capital cost, reactor life, interest rates, gas cleanup costs, and carbon credits are needed. The fundamental challenge to AD deployment in the US is the relatively low commercial energy prices.

Chapter 3 modeled costs for industrial fermentation processes for biorenewable chemical production. The field of metabolic engineering has led to tremendous advances in microbial strains used for industrial fermentation. Scientists are able to target the genes that control cellular functions to improve the specific growth rates, yield, productivities, and substrate concentration; however, as one or more of these variables is adjusted, there are often tradeoffs in other variables. In a competitive industry where process economics determine technology deployment, understanding the economic impact of these kinetic tradeoffs is vital at the early stages of development. The FEMT was developed to evaluate the cost structures and tradeoffs in industrial fermentation systems. Results showed that the

yield, fraction of the product in the biomass, and substrate concentration have the greatest impact on changes in the product cost. Using FEMT we can illustrate that increases in substrate concentration resulting in decreases in the maximum specific growth rate result have a greater impact on the production cost than increases in maximum specific growth rate leading to reductions in the substrate concentration. Additionally, using fermentation for production of commodity chemicals will require high maximum specific growth rates and substrate concentrations as well as low separation costs. Research focusing on these areas is likely to have the greatest impact on process economics. FEMT also provides a consistent reporting methodology that can be used by metabolic engineers for increased continuity in literature.

Another important take-away from this research is best practices in spreadsheet model development. S-FAAD was developed using in-cell computations while FEMT was developed using VBA to complete and output all calculations results. There are advantages and disadvantages to each of these methodologies. While in-cell computations allow for immediate results and allow the user to see how the calculations are structured, they are not well suited for models with varying levels of analysis and can be changed by the user. VBA allows for a single interface to be used for multiple levels of analysis and gives the designer greater power over the model; however, any change in the analysis or results that are output requires additional time and programming that is not always trivial. For models that are well-defined and that have specific sets of requirements using VBA to complete all calculations is recommended; however, in situations where the inputs, outputs, and analysis method may change in-cell computations are recommended.

Future Work

The use of biorenewable resources and products relies heavily on process economics. Evaluating the cost structures for different bioprocesses is an important step in deepening our understanding of different processes; however, additional work is needed to improve models and the technology at hand.

Our discussion of anaerobic digestion is limited to plug-flow digesters on dairy farms. While this type of digester provides a good foundation for understanding AD economics since it is well-documented and more widely used than other digesters, evaluating different substrates and digesters would be useful. In addition, our model did not incorporate kinetics. Using a kinetic model to calculate the biogas production for different retention times as well as different influent strengths would enhance the capabilities of the model. Additionally, research is needed in the area of reliability and digester construction for AD. The capital cost of AD systems remains high and is the most promising area for reducing the production cost. In addition, reliability remains an issue that hampers AD economics on farms. Developing training programs for AD operators or evaluating different digester designs to improve the life and reliability of a digester would improve the economic outlook for the technology.

One of the challenges in modeling industrial fermentation for biorenewable chemicals is the lack of available cost and kinetics information. Many companies have proprietary processes and do not share or publish production cost data, making it difficult to validate cost models. The USDA has published studies on ethanol production in the US using surveys for different companies to report data without exposing company information. A similar study surveying companies that currently produce biorenewable chemicals would provide baseline data that could be used in academia to strengthen existing cost models.

In addition, comparing FEMT to an ASPEN model for a specific process and completing statistical analysis to determine which variables in the ASPEN model can be removed without compromising an order-of-magnitude cost estimate would validate the use of simpler models like FEMT.

Finding a balance between overly simplified models and complex models is another challenge. The FEMT is very simple and easy to use; however, adding a slightly more complex kinetic model to the FEMT would enable it to more accurately portray industrial operating systems.

As we continue to deplete our fossil-fuel resource base, finding alternative resources for chemical, energy, and transportation fuel production is vital. Fermentation processes can be used to offset fossil-fuels and have been used on farms and in industry in the past. To exploit the benefits of fermentation, developing cost competitive products is necessary.

In the case of AD, evaluating different technologies to reduce the capital cost for installed systems appears to be one of the most promising methods for reducing the production cost. In addition, policies that reduce interest rates for farmers would also help improve deployment rates.

In industrial fermentation processes, economic evaluations should be introduced early on in the research and design stages to develop more targeted research projects that result in industrial deployment.

APPENDIX

Section A: S-FAAD MODEL CODE AND IMAGES

S-FAAD Figure and Code Description

Figures A1-A2 below illustrates different spreadsheet tabs in the interface for S-FAAD. Figure A1 shows the main page which includes primary inputs and outputs, a single variable analysis program, simulation table, cost structure and sensitivity analysis programs, and a multiple variable test. Figure A2 shows the odor and GHG calculations page.

Code for each of these modules is included below the figures.

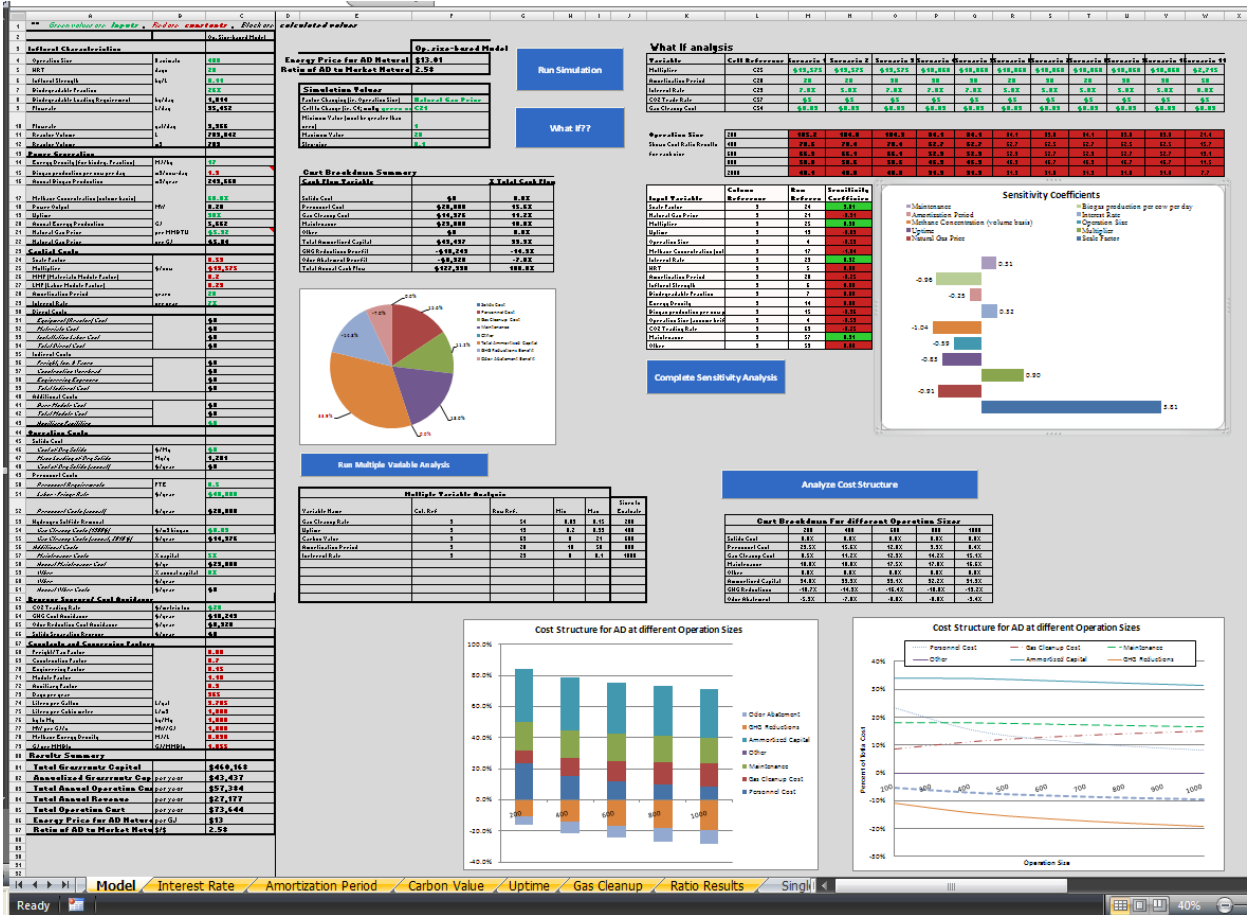


Figure A1. S-FAAD Main Page Interface

	A	B	C
1	Odor Reduction		
2	Operation Size (heifers)		1000
3	Average Home Price		\$100,000
4	Average Lot Size	acre	0.35
5	Average Depreciation Life	year	50
6	Amortized Property Cost	\$/acre/year	\$5,714
7	Area Equation Slope	mile	3.65E-04
8	Percent Reduction in Odor from AD		84%
9	Impacted Land Area (sq. miles; No AD - AD)	sq. miles	0.31
10	Acres per sq. Mile	acres/mi ²	640
11	Impacted Land Area (acres)	acres	195
12	Property Devaluation due to Odor		2%
13	Annual Cost Avoidance		\$22,320.37
14			
15	GHG Emission Calculations		
16	Baseline Emissions Calculations		
17	TVS	kg/cow-day	5.7
18	Biogas Production	m ³ /cow-day	1.9
19	Biogas Methane Concentration	by volume	60%
20	Daily Methane Production	m ³ /cow-day	1.14
21	Bo	m ³ /kg TVS excreted	0.20
22	MCF (Waste Management Sys. Correction Factor)		0.23
23	Farm Size		1000
24	Baseline VS Excreted	kg/year	2,080,500
25	Baseline Methane Emissions	kg CH ₄ /year	63,355
26	AD Emissions Calculations		
27	AD Methane Production	kg/year	447,516
28	Collection Efficiency		0.99
29	Destruction Efficiency		0.98
30	AD Methane Emissions (leakage)	kg/year	13,336
31	AD Emissions Reductions		
32	Annual Methane Reduction	kg/year	50,019
33	CO ₂ Multiplier		21
34	Annual GHG Reduction	kg CO ₂ e/year	1,050,408
35	kg per metric ton	kg/ metric ton	1,000
36	CO ₂ Trading Rate	\$/ton	\$20
37	Annual Cost Savings	\$	\$21,008
38	Fossil Fuel Offset		
39	Annual Methane Production	L/year	624,150,000
40	Methane Density	kg/L	0.00072
41	CO ₂ Conversion Factor	MW CO ₂ /MW CH ₄	2.75
42	Annual CO ₂ Emissions	kg/year	1,230,668
43	Annual CO ₂ Emissions	metric ton/year	1,231
44	Annual Cost Savings		\$24,613.36
45			
46			
47			
48			
49			
50			

Summary of Recent Changes | Model | Capital cost | Auxiliary Calcula

Ready

Figure A2. Odor and GHG Interface

Code for Main Page

```
Private Sub CommandButton1_Click()
' This code is designed to read in values provided by the user in the Simulation Values
Section.
' The code then changes the model accordingly and reads in the change in energy price and
ratio of AD to Market Nat Gas Price
' Finally data is output to the simulation results tab and used to create the graph seen on the
user interface.
' Author: Carol Faulhaber, Created 1/07/2010
```

```
'Clear Contents from Previous Simulation
Worksheets("Simulation Results").Range("A1:H2000").ClearContents
```

```
ChangeFactor2 = Worksheets("Model").Range("F8").Value
cell2 = Worksheets("Model").Range("F9").Value
MinVal2 = Worksheets("Model").Range("F10").Value
MaxVal2 = Worksheets("Model").Range("F11").Value
StepSize2 = Worksheets("Model").Range("F12").Value
```

```
B = 2
```

```
'Start and MinVal
InputVariable2 = MinVal2
```

```
Do While InputVariable2 < MaxVal2
```

```
    'InputVariable is output to model is designated cell
    Worksheets("Model").Range(cell2) = InputVariable2
```

```
    'Resulting Output is given a variable name
    Out3 = Worksheets("Model").Range("E4").Value
    Out4 = Worksheets("Model").Range("E5").Value
    NRGPrice2 = Worksheets("Model").Range("F4").Value
    NRGRatio2 = Worksheets("Model").Range("F5").Value
```

```
    'Results and InputVariable are output to simulation results tab
    Worksheets("Simulation Results").Range("A1") = ChangeFactor2
    Worksheets("Simulation Results").Range("B1") = Out3
    Worksheets("Simulation Results").Range("C1") = Out4
    Worksheets("Simulation Results").Range("A" & B) = InputVariable2
    Worksheets("Simulation Results").Range("B" & B) = NRGPrice2
    Worksheets("Simulation Results").Range("C" & B) = NRGRatio2
```

```
    B = B + 1
    InputVariable2 = InputVariable2 + StepSize2
```

Loop

End Sub

Private Sub CommandButton2_Click()

'This performs a What if analysis allowing to the user to vary multiple variables at once and see results

'Author: Carol Faulhaber, March 16, 2010

Dim Scenario(1000) As Double, CellRef(1000) As String, InputChange(10000) As String, OriginalValue(10000) As Variant

Dim OpSize(1000) As Integer, Ratio(1000) As Double

'Loops through columns until out of scenarios to test

'set a to M

a = 13

Do While IsEmpty(Worksheets("Model").Cells(5, a)) = False

 'loop through values to change

 B = 5

 c = 1

 Do While IsEmpty(Worksheets("Model").Cells(B, a)) = False

 'InputChange Variable name

 InputChange(c) = Worksheets("Model").Cells(B, 13).Offset(0, -2).Value

 CellRef(c) = Worksheets("Model").Cells(B, 13).Offset(0, -1).Value

 Scenario(c) = Worksheets("Model").Cells(B, a).Value

 'statement to read in initial values before making changes

 'Only reads for fist loop through

 If a = 13 Then

 If Worksheets("Model").Range(CellRef(c)).HasFormula = "True" Then

 OriginalValue(c) = Worksheets("Model").Range(CellRef(c)).Formula

 Else

 OriginalValue(c) = Worksheets("Model").Range(CellRef(c)).Value

 End If

 Else

 End If

 Worksheets("Model").Range(CellRef(c)).Value = Scenario(c)

 c = c + 1

 B = B + 1

Loop

'Second Loop to go through Op Sizes

d = 1

f = B + 1

Do While IsEmpty(Worksheets("Model").Cells(f, 12)) = False

OpSize(d) = Worksheets("Model").Cells(f, 12).Value

Worksheets("Model").Range("C4").Value = OpSize(d)

Ratio(d) = Worksheets("Model").Range("F5").Value

Worksheets("Model").Cells(f, a).Value = Ratio(d)

'colors cells red or green based on > or < 1

If Ratio(d) < 1 Then

Worksheets("Model").Cells(f, a).Interior.Color = RGB(50, 205, 50)

Else

Worksheets("Model").Cells(f, a).Interior.Color = RGB(200, 34, 34)

End If

f = f + 1

Loop

a = a + 1

Loop

For e = 1 To c - 1

Worksheets("Model").Range(CellRef(e)).Value = OriginalValue(e)

Next e

End Sub

Private Sub CommandButton3_Click()

'Title: Multiple Variable Analysis

'Author: Carol Faulhaber

'Last Updated: April 11, 2011

'Description: This program is designed to run through multiple sizes and variable ranges.

'100 values are evaluated for each variable range listed by the user.

'The resulting outputs are recorded and graphs are generated for each size specified.

'Name and dimension variables

'option explicit has not been used for this program, so counters are not dimensioned

```
Dim TestVar(1000) As Double, ColRef As Integer, RowRef As Integer, MinVal As Double,
MaxVal As Double, Size(10) As Integer
```

```
'Clear previous values
Worksheets("Ratio Results").Range("A1:BB105").ClearContents
```

```
'Establish the beginning row corresponding to values in the table
RowCount = 53
```

```
'This will run the program until no more values are found in the table, so the user can specify
additional variables for evaluation
```

```
ColCounter = 1 'establishes first column to output results into
Do While IsEmpty(Worksheets("Model").Cells(RowCount, 5)) = False
```

```
'Read in the first set of variables for the multiple variable analysis
VarName = Worksheets("Model").Cells(RowCount, 5).Value
ColRef = Worksheets("Model").Cells(RowCount, 6).Value
RowRef = Worksheets("Model").Cells(RowCount, 7).Value
MinVal = Worksheets("Model").Cells(RowCount, 8).Value
MaxVal = Worksheets("Model").Cells(RowCount, 9).Value
```

```
'Record initial value in cell so that the variable after the simulation can be returned to the
initial value
```

```
InitialVarVal = Worksheets("Model").Cells(RowRef, ColRef).Value
```

```
'begin loop to run through each size
```

```
SizeCounter = 53
```

```
Do While IsEmpty(Worksheets("Model").Cells(SizeCounter, 10)) = False
```

```
'Change size based on value
```

```
DairySize = Worksheets("Model").Cells(SizeCounter, 10).Value
```

```
Worksheets("Model").Range("C4").Value = DairySize
```

```
'Create array of testing values based on min and max value with 100 variables
```

```
Call Simulation(TestVar(), MinVal, MaxVal)
```

```
'Loop through each value and record result
```

```
For a = 1 To 100
```

```
'change variable of interest
```

```
Worksheets("Model").Cells(RowRef, ColRef).Value = TestVar(a)
```

```
'Record resulting ratio
```

```
MCR = Worksheets("Model").Range("F5").Value
```

```
'Output Results and titles
```



```

Worksheets("Ratio Results").Cells(1, ColCounter).Value = VarName
Worksheets("Ratio Results").Cells(1, ColCounter + 1).Value = "MCR for " &
DairySize
Worksheets("Ratio Results").Cells(a + 1, ColCounter).Value = TestVar(a)
Worksheets("Ratio Results").Cells(a + 1, ColCounter + 1).Value = MCR

```

```

Next a

```

```

ColCounter = ColCounter + 2 'add 2 because first col is always test variable and second
col is always result

```

```

SizeCounter = SizeCounter + 1
Loop

```

```

'Return test variable to initial value so that testing is standardized
Worksheets("Model").Cells(RowRef, ColRef).Value = InitialVarVal

```

```

RowCount = RowCount + 1
Loop

```

```

End Sub

```

```

Public Sub Simulation(ByRef SimArray() As Double, ByVal Min, ByVal Max)
'Subroutine Description: This subroutine takes in an empty array, the minimum and max
values and creates an array with 100 values

```

```

Dim NumValues As Integer

```

```

NumValues = 100

```

```

'create an array for 100 values that can be used to run simulations

```

```

stepsize = (Max - Min) / NumValues

```

```

B = 1

```

```

For a = Min To Max Step stepsize

```

```

    SimArray(B) = a

```

```

    B = B + 1

```

```

Next a

```

```

End Sub

```

```

Private Sub CommandButton4_Click()

```

```

'Description: Completes Sensitivity Analysis using sensitivity coefficients as described in
Hamby (2004).

```

```

'Author: Carol Faulhaber

```

'Date Updated: 4/11/2011

'Read in the initial MCR Value

MCR = Worksheets("Model").Cells(5, 6).Value

RowCount = 18 'based on location of table

'Loop through variables in table until no more are listed

Do While IsEmpty(Worksheets("Model").Cells(RowCount, 11).Value) = False

 'Read in values from table

 ColRef = Worksheets("Model").Cells(RowCount, 12).Value

 RowRef = Worksheets("Model").Cells(RowCount, 13).Value

 'Read in initial variable value and apply change

 InitialVarVal = Worksheets("Model").Cells(RowRef, ColRef).Value

 VarChanged = InitialVarVal * 1.1

 Worksheets("Model").Cells(RowRef, ColRef).Value = VarChanged

 MCRChanged = Worksheets("Model").Cells(5, 6).Value

 'Calculate Sensitivity Coefficient

 ChangeIn = 0.1

 ChangeOut = (MCRChanged - MCR) / MCR

 SensitivityCoef = ChangeOut / ChangeIn

 'Output Result to table and color based on sign

 Worksheets("Model").Cells(RowCount, 14).Value = SensitivityCoef

 If SensitivityCoef > 0 Then

 Worksheets("Model").Cells(RowCount, 14).Interior.Color = RGB(50, 205, 50)

 Else

 Worksheets("Model").Cells(RowCount, 14).Interior.Color = RGB(200, 34, 34)

 End If

 'Replace initial value

 Worksheets("Model").Cells(RowRef, ColRef).Value = InitialVarVal

 RowCount = RowCount + 1

Loop

End Sub

Private Sub CommandButton5_Click()

 'Title: Cost Structure Analysis

 'Author: Carol Faulhaber

 'Date Updated: April 13, 2011

'Description: Analyzes percent of total cost for different sizes

'Dimension Variables

Dim SizeChange As Integer

'Loop to go through each size

SizeCounter = 13

Do While IsEmpty(Worksheets("Model").Cells(54, SizeCounter).Value) = False

 'Read in the size and then input it into the model

 SizeChange = Worksheets("Model").Cells(54, SizeCounter).Value

 Worksheets("Model").Range("C4").Value = SizeChange

 'Read in values and paste them

 Worksheets("Model").Range("G17:G24").Select

 Selection.Copy

 Worksheets("Model").Cells(55, SizeCounter).Select

 Selection.PasteSpecial Paste:=xlPasteValues, Operation:=xlNone, SkipBlanks _
 :=False, Transpose:=False

 SizeCounter = SizeCounter + 1

Loop

End Sub

APPENDIX

Section B: FEMT MODEL CODE AND IMAGES

Description of Figures and Code

When FEMT was developed, three levels of analysis were completed in increasing complexity. The Level 3 (L3) analysis, discussed in Chapter 3 is discussed in further detail below. Three figures, A1, A2, and A3 are presented below to illustrate the interface of the FEMT L3 analysis. Figure A1 illustrates the inputs page for the analysis. As shown in figure A1, in addition to the inputs selected, the user can also adjust the uncertainty in each input. Additionally, the sensitivity coefficients are also displayed next to each variable. Figure A2 shows the intermediate calculations page. Figure A3 shows the results page. As shown in Figure A3, graphs for each input variable are displayed based on the uncertainty selected by the user. The x-axis range for each graph is determined using the uncertainty selected by the user in terms of plus or minus “X”%. Below the figures, the code used to complete all model calculations is displayed.

	A	B	C	D	E	F	G
1							
2	Run Program			The Fermentation Economic Modeling Tool provides an order of magnitude estimate for the cost to produce a chemical of interest from glucose via fermentation. The variables considered in this cost include the feedstock cost, reactor cost, and separation cost. To use the model, enter values into the yellow cells and then press "Run Program". Intermediate calculations as well as graphs and a sensitivity analysis are automatically completed when the button is pressed.			
3							
4							
5	Inputs						
6							
7	<u>Feedstock Cost Inputs</u>	Reference Values	Testing Values	Uncertainty (%)	Sensitivity Coefficient	Units	
8	Glucose Cost	\$0.12	\$0.10	15%	0.157	\$/kg glucose	
9	f_{px}	0.70	0.6	15%	-1.003		
10	Y_{xs}	0.50	0.7	15%	-1.009		
11							
12	<u>Fermenter Rental Rate Inputs</u>						
13	Fermenter Volume, V	500	100			cubic meters	
14	Interest Rate	15%	15%	15%	0.480	per year	
15	Reactor Life	10	10	15%	-0.389	years	
16	Downtime between runs	12	12	%		hrs	
17	K_s	1.0	5	15%	0.052	g/L (kg/m ³)	
18	S_0	100	25	15%	-0.762	g/L (kg/m ³)	
19	X_0	0.5	0.5	15%	-0.106	g/L (kg/m ³)	
20	μ_m	0.3	0.4	15%	-0.389	per hour	
21							
22	<u>Separation Inputs</u>						
23	Separation	80%	80%	15%	0.328	% relative to reactor cost	
24							
25	1						
26	Target Product Price		\$0.75			\$/kg	
27	Other		25%	15%	0.102	% relative to reactor cost	
28							

Validation Dat **Inputs** Intermediate Calculations Results Storage SimTable PieCharts Sensitivity

Ready

Figure A1. L3 Inputs Page.

	A	B	C	D	E	F	G	H	I		
2											
3											
4		Glucose Cost	}	Feedstock Cost, \$/kg prod.	\$0.24						
5		f_{pk}									
6		Y_{xz}									
7											
8											
9		Volume	}	Interest Rate	\$1,210,589	}	Amortized Capital Cost	\$241,212			
10		Multiplier		Reactor Cost							
11		Scale Factor		Reactor Life							
12											
13											
14		K_s	}	τ , hrs	10.2	}	Corrected τ				
15		S_o									
16		X_o					Downtime between loading			22.2	
17		μ_m									
18											
19											
20		Corrected τ	}	Production Rate, kg/hr	46.2	}	Annual Production Rate, kg/yr				
21		X_r									
22		f_{pk}					Hours per year			388,054	
23		Fermenter Volume, V									
24		Reactor Cost									
25											
26											
27		X_r	}	Productivity, g/L-hr	1.00						
28		τ									
29		f_{pk}									
30											
31											
32		Y_{xz}	}	X_r	17.10						
33		S_o									
34		X_o									
35											
36											
37		X_o	}	Innoculum	2.92%						
38		X_r									
39											
40											
41		corrected τ	}	Productivity, g/L-hr	0.46						
42		f_{pk}									
43											
44											

Figure 2A. L3 Intermediate Calculations Page.

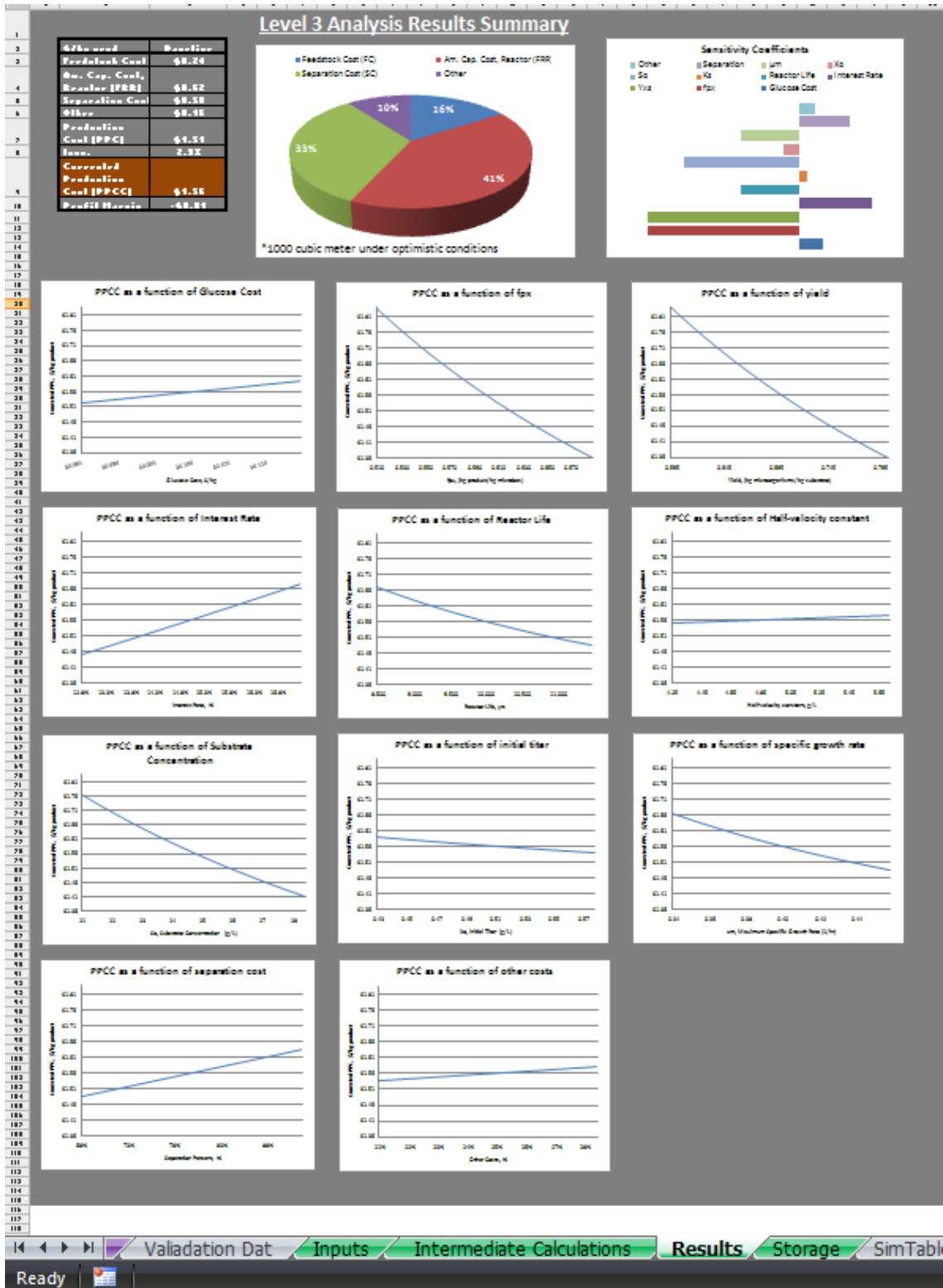


Figure 3A. L3 Results Page.

Level 3 Code

Private Sub CommandButton1_Click()

'Program Author: Carol Faulhaber

'Date: 1.27.11

'Program Description: this program completes a level 3 kinetic analysis and outputs results to the results page

'Dimension variables

Dim GArray(1000) As Double, G As Double, GU As Double, Gbest As Double, Gworst As Double

Dim PBFArray(1000) As Double, PBF As Double, PBFU As Double, PBFbest As Double, PBFworst As Double

Dim YArray(1000) As Double, Y As Double, YU As Double, Ybest As Double, Yworst As Double

Dim FC As Double, FCbest As Double, FCworst As Double, FCSim As Double

Dim V As Double, VU As Double

Dim IR As Double, IRU As Double, IRBest As Double, IRWorst As Double, IRArray(1000) As Double

Dim RL As Double, RLU As Double, RLbest As Double, RLworst As Double, RLArray(1000) As Double

Dim Xf As Double, XfU As Double, XfBest As Double, XfWorst As Double, XfArray(1000) As Double

Dim Tau As Double, TauU As Double, TauBest As Double, TauWorst As Double, TauArray(1000) As Double

Dim RC As Double, RCbest As Double, RCworst As Double

Dim FRR As Double, FRRBest As Double, FRRWorst As Double

Dim So As Double, SoU As Double, SoArray(1000) As Double

Dim Xo As Double, XoU As Double, XoArray(1000) As Double

Dim ks As Double, ksU As Double

Dim um As Double, umU As Double, umArray(1000) As Double

Dim sep As Double, sepU As Double, sepArray(1000) As Double

Dim inoc As Double, inocU As Double, inocArray(1000) As Double

Dim Downtime As Double

Dim Productivity As Double

Dim GPPCArray(1000) As Double, PBFPPCArray(1000) As Double, YPPCArray(1000) As Double, IRPPCArray(1000) As Double, RLPPCArray(1000) As Double

Dim XfPPCArray(1000) As Double, TauPPCArray(1000) As Double, RCPPCArray(1000) As Double, SoPPCArray(1000) As Double, XoPPCArray(1000) As Double

Dim ksPPCArray(1000) As Double, umPPCArray(1000) As Double, sepPPCArray(100) As Double

Dim FCArray(1000) As Double, FRRArray(1000) As Double, TotSepArray(1000) As Double, RCArray(1000) As Double

Dim CorrectedTauArray(1000) As Double, ksArray(1000) As Double, inocTotArray(1000) As Double

```

Dim TPP As Double, TPPU As Double, TPPArray(1000) As Double
Dim NRG As Double, NRGU As Double, NRGArray(1000) As Double
Dim Lab As Double, LabU As Double, LabArray(1000) As Double
Dim UPC As Double, UPCU As Double, UPCArray(1000) As Double
Dim Other As Double, TotOther As Double, TotOtherArray(10000) As Double,
OtherArray(1000) As Double
Dim OtherPPCArray(10000) As Double

```

```
'Clear intermediate calcs from previous run
```

```
Worksheets("Intermediate Calculations").Range("E5:E45").ClearContents
```

```
Worksheets("Intermediate Calculations").Range("H10").ClearContents
```

```
Worksheets("Intermediate Calculations").Range("G16").ClearContents
```

```
Worksheets("Intermediate Calculations").Range("G23").ClearContents
```

```
'Read in variables for L3 Analysis
```

```
G = Worksheets("Inputs").Range("C8").Value 'glucose cost
```

```
GU = Worksheets("Inputs").Range("D8").Value 'uncertainty in glucose cost
```

```
PBF = Worksheets("Inputs").Range("C9").Value 'product in biomass
```

```
PBFU = Worksheets("Inputs").Range("D9").Value 'uncertainty in product in biomass
```

```
Y = Worksheets("Inputs").Range("C10").Value 'yield
```

```
YU = Worksheets("Inputs").Range("D10").Value 'yield uncertainty
```

```
V = Worksheets("Inputs").Range("C13").Value 'reactor volume
```

```
VU = Worksheets("Inputs").Range("D13").Value 'volume uncertainty
```

```
IR = Worksheets("Inputs").Range("C14").Value 'interest rate
```

```
IRU = Worksheets("Inputs").Range("D14").Value 'interest rate uncertainty
```

```
RL = Worksheets("Inputs").Range("C15").Value 'reactor life
```

```
RLU = Worksheets("Inputs").Range("D15").Value 'reactor life uncertainty
```

```
ks = Worksheets("Inputs").Range("C17").Value 'half-life velocity constant
```

```
ksU = Worksheets("Inputs").Range("D17").Value 'half-life velocity uncertainty
```

```
So = Worksheets("Inputs").Range("C18").Value 'rate-limiting substrate concentration
```

```
SoU = Worksheets("Inputs").Range("D18").Value 'substrate concentration uncertainty
```

```
Xo = Worksheets("Inputs").Range("C19").Value 'initial cell concentration
```

```
XoU = Worksheets("Inputs").Range("D19").Value 'cell concentration uncertainty
```

```
um = Worksheets("Inputs").Range("C20").Value 'maximum growth rate constant
```

```
umU = Worksheets("Inputs").Range("D20").Value 'growth rate constant uncertainty
```

```
sep = Worksheets("Inputs").Range("C23").Value 'separation costs
```

```
sepU = Worksheets("Inputs").Range("D23").Value 'sep cost uncertainty
```

```
Downtime = Worksheets("inputs").Range("C16").Value 'downtime between loadings
```

```
TPP = Worksheets("inputs").Range("C26").Value
```

```
Other = Worksheets("inputs").Range("C27").Value
```

```
OtherU = Worksheets("inputs").Range("D27").Value
```

```
'-----Complete FC Calculations. For L3 analysis PPC=FC+FR+SC-----
```

```
'Calculations output to the inputs page
```

$\text{Tau} = \text{LogisticEq}(ks, Y, S_o, X_o, um)$
 $\text{Worksheets}(\text{"Intermediate Calculations"}).\text{Range}(\text{"E15"}).\text{Value} = \text{Tau}$
 $\text{CorrectedTau} = \text{Tau} + \text{Downtime}$
 $\text{Worksheets}(\text{"Intermediate Calculations"}).\text{Range}(\text{"G16"}).\text{Value} = \text{CorrectedTau}$

'Titer Calculation
 $X_f = 0.95 * ((S_o * Y) + X_o)$
 $\text{Worksheets}(\text{"Intermediate Calculations"}).\text{Range}(\text{"E33"}).\text{Value} = X_f$

'productivity
 $\text{Productivity} = \text{PBF} * (X_f / \text{Tau})$
 $\text{Worksheets}(\text{"Intermediate Calculations"}).\text{Range}(\text{"E28"}).\text{Value} = \text{Productivity}$

'corrected productivity
 $\text{ProductivityCorrected} = \text{PBF} * (X_f / \text{CorrectedTau})$
 $\text{Worksheets}(\text{"Intermediate Calculations"}).\text{Range}(\text{"E42"}).\text{Value} = \text{ProductivityCorrected}$

'inoculum
 $\text{inoc} = X_o / X_f$
 $\text{Worksheets}(\text{"Intermediate Calculations"}).\text{Range}(\text{"E38"}).\text{Value} = \text{inoc}$

'-----Basecase Calculations

'FC basecase
 $\text{FC} = \text{FeedstockCost}(G, \text{PBF}, Y)$
 $\text{Worksheets}(\text{"Results"}).\text{Range}(\text{"C3"}).\text{Value} = \text{FC}$
 $\text{Worksheets}(\text{"Intermediate Calculations"}).\text{Range}(\text{"E5"}).\text{Value} = \text{FC}$

'FRR
 $\text{RC} = \text{ReactorCost}(V, \text{IR}, \text{RL})$
 $\text{Worksheets}(\text{"Intermediate Calculations"}).\text{Range}(\text{"H10"}).\text{Value} = \text{RC}$
 $\text{Tau} = \text{LogisticEq}(ks, Y, S_o, X_o, um)$
 $\text{CorrectedTau} = \text{Tau} + \text{Downtime}$
 $X_f = 0.95 * ((S_o * Y) + X_o)$
 $\text{FRR} = \text{FermentorRRate}(\text{RC}, X_f, \text{PBF}, V, \text{CorrectedTau})$
 $\text{Worksheets}(\text{"Results"}).\text{Range}(\text{"C4"}).\text{Value} = \text{FRR}$

'Sep
 $\text{TotSep} = \text{sep} * \text{FRR}$
 $\text{Worksheets}(\text{"Results"}).\text{Range}(\text{"C5"}).\text{Value} = \text{TotSep}$

'Other
 $\text{TotOther} = \text{Other} * \text{FRR}$
 $\text{Worksheets}(\text{"Results"}).\text{Range}(\text{"C6"}).\text{Value} = \text{TotOther}$

'PPC

```

PPC = FC + FRR + TotSep + TotOther
Worksheets("Results").Range("C7").Value = PPC

```

```

'Inoc
inoc = Xo / Xf
Worksheets("Results").Range("C8").Value = inoc

```

```

'CorrectedPPC
CorrectedPPC = PPC / (1 - inoc)
Worksheets("Results").Range("C9").Value = CorrectedPPC

```

```

'Profit margin
Pmargin = TPP - CorrectedPPC
Worksheets("Results").Range("C10").Value = Pmargin

```

```

'-----Begin Simulations-----

```

```

'Assign Arrays for each input. Each array will contain 100 values and is based on the
uncertainty

```

```

Call Simulation(GArray(), G, GU)
Call Simulation(PBFArray(), PBF, PBFU)
Call Simulation(YArray(), Y, YU)
Call Simulation(IRArray(), IR, IRU)
Call Simulation(RLArray(), RL, RLU)
Call Simulation(ksArray(), ks, ksU)
Call Simulation(SoArray(), So, SoU)
Call Simulation(XoArray(), Xo, XoU)
Call Simulation(umArray(), um, umU)
Call Simulation(sepArray(), sep, sepU)
Call Simulation(OtherArray(), Other, OtherU)

```

```

'Loop through all data and output results to storage tab
For i = 1 To 100

```

```

    'glucose cost
    FCArray(i) = FeedstockCost(GArray(i), PBF, Y)
    inoctot = Xo / Xf
    GPPCArray(i) = (FCArray(i) + FRR + TotSep + TotOther) / (1 - inoc) 'other
    Worksheets("Storage").Cells(i + 1, 1).Value = GArray(i)
    Worksheets("Storage").Cells(i + 1, 2).Value = GPPCArray(i)

```

```

    'fraction of the biomass in the product
    FCArray(i) = FeedstockCost(G, PBFArray(i), Y)
    FRRArray(i) = FermentorRRate(RC, Xf, PBFArray(i), V, CorrectedTau)
    TotSepArray(i) = sep * FRRArray(i)
    TotOtherArray(i) = Other * FRRArray(i) 'other

```

$$\text{PBFPPCArray}(i) = (\text{FCArray}(i) + \text{FRRArray}(i) + \text{TotSepArray}(i) + \text{TotOtherArray}(i)) / (1 - \text{inocTot})$$
 'other
 Worksheets("Storage").Cells(i + 1, 3).Value = PBFArray(i)
 Worksheets("Storage").Cells(i + 1, 4).Value = PBFPPCArray(i)

'yield

$$\text{FCArray}(i) = \text{FeedstockCost}(G, \text{PBF}, \text{YArray}(i))$$

$$\text{TauArray}(i) = \text{LogisticEq}(ks, \text{YArray}(i), \text{So}, \text{Xo}, \text{um})$$

$$\text{CorrectedTauArray}(i) = \text{Tau} + \text{Downtime}$$

$$\text{XfArray}(i) = 0.95 * ((\text{So} * \text{YArray}(i)) + \text{Xo})$$

$$\text{FRRArray}(i) = \text{FermentorRRate}(\text{RC}, \text{XfArray}(i), \text{PBF}, \text{V}, \text{CorrectedTauArray}(i))$$

$$\text{TotSepArray}(i) = \text{sep} * \text{FRRArray}(i)$$

$$\text{TotOtherArray}(i) = \text{Other} * \text{FRRArray}(i)$$
 'other

$$\text{inocTotArray}(i) = \text{Xo} / \text{XfArray}(i)$$

$$\text{YPPCArray}(i) = (\text{FCArray}(i) + \text{FRRArray}(i) + \text{TotSepArray}(i) + \text{TotOtherArray}(i)) / (1 - \text{inocTotArray}(i))$$
 'other
 Worksheets("Storage").Cells(i + 1, 5).Value = YArray(i)
 Worksheets("Storage").Cells(i + 1, 6).Value = YPPCArray(i)

'interest rate

$$\text{RCArray}(i) = \text{ReactorCost}(\text{V}, \text{IRArray}(i), \text{RL})$$

$$\text{FRRArray}(i) = \text{FermentorRRate}(\text{RCArray}(i), \text{Xf}, \text{PBF}, \text{V}, \text{CorrectedTau})$$

$$\text{TotSepArray}(i) = \text{sep} * \text{FRRArray}(i)$$

$$\text{TotOtherArray}(i) = \text{Other} * \text{FRRArray}(i)$$
 'other

$$\text{IRPPCArray}(i) = (\text{FC} + \text{FRRArray}(i) + \text{TotSepArray}(i) + \text{TotOtherArray}(i)) / (1 - \text{inocTot})$$
 'other
 Worksheets("Storage").Cells(i + 1, 7).Value = IRArray(i)
 Worksheets("Storage").Cells(i + 1, 8).Value = IRPPCArray(i)

'reactor life

$$\text{RCArray}(i) = \text{ReactorCost}(\text{V}, \text{IR}, \text{RLArray}(i))$$

$$\text{FRRArray}(i) = \text{FermentorRRate}(\text{RCArray}(i), \text{Xf}, \text{PBF}, \text{V}, \text{CorrectedTau})$$

$$\text{TotSepArray}(i) = \text{sep} * \text{FRRArray}(i)$$

$$\text{TotOtherArray}(i) = \text{Other} * \text{FRRArray}(i)$$
 'other

$$\text{RLPPCArray}(i) = (\text{FC} + \text{FRRArray}(i) + \text{TotSepArray}(i) + \text{TotOtherArray}(i)) / (1 - \text{inocTot})$$
 'other
 Worksheets("Storage").Cells(i + 1, 9).Value = RLArray(i)
 Worksheets("Storage").Cells(i + 1, 10).Value = RLPPCArray(i)

'half-velocity constant

$$\text{TauArray}(i) = \text{LogisticEq}(ks\text{Array}(i), \text{Y}, \text{So}, \text{Xo}, \text{um})$$

$$\text{CorrectedTauArray}(i) = \text{TauArray}(i) + \text{Downtime}$$

$$\text{XfArray}(i) = 0.95 * ((\text{So} * \text{Y}) + \text{Xo})$$

$$\text{FRRArray}(i) = \text{FermentorRRate}(\text{RC}, \text{XfArray}(i), \text{PBF}, \text{V}, \text{CorrectedTauArray}(i))$$

$$\text{TotSepArray}(i) = \text{sep} * \text{FRRArray}(i)$$

$$\text{TotOtherArray}(i) = \text{Other} * \text{FRRArray}(i)$$
 'other

ksPPCArray(i) = (FC + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) / (1 - inocticot) 'other

Worksheets("Storage").Cells(i + 1, 11).Value = ksArray(i)

Worksheets("Storage").Cells(i + 1, 12).Value = ksPPCArray(i)

'substrate concentration

TauArray(i) = LogisticEq(ks, Y, SoArray(i), Xo, um)

CorrectedTauArray(i) = TauArray(i) + Downtime

XfArray(i) = 0.95 * ((SoArray(i) * Y) + Xo)

FRRArray(i) = FermentorRRate(RC, XfArray(i), PBF, V, CorrectedTauArray(i))

TotSepArray(i) = sep * FRRArray(i)

TotOtherArray(i) = Other * FRRArray(i) 'other

inocTotArray(i) = Xo / XfArray(i)

SoPPCArray(i) = (FC + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) / (1 - inocticot) 'other

Worksheets("Storage").Cells(i + 1, 13).Value = SoArray(i)

Worksheets("Storage").Cells(i + 1, 14).Value = SoPPCArray(i)

'initial titer

TauArray(i) = LogisticEq(ks, Y, So, XoArray(i), um)

CorrectedTauArray(i) = TauArray(i) + Downtime

XfArray(i) = 0.95 * ((So * Y) + XoArray(i))

FRRArray(i) = FermentorRRate(RC, XfArray(i), PBF, V, CorrectedTauArray(i))

TotSepArray(i) = sep * FRRArray(i)

TotOtherArray(i) = Other * FRRArray(i) 'other

inocTotArray(i) = XoArray(i) / XfArray(i)

XoPPCArray(i) = (FC + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) / (1 - inocTotArray(i)) 'other

Worksheets("Storage").Cells(i + 1, 15).Value = XoArray(i)

Worksheets("Storage").Cells(i + 1, 16).Value = XoPPCArray(i)

'max specific growth rate

TauArray(i) = LogisticEq(ks, Y, So, Xo, umArray(i))

CorrectedTauArray(i) = TauArray(i) + Downtime

XfArray(i) = 0.95 * ((So * Y) + Xo)

FRRArray(i) = FermentorRRate(RC, XfArray(i), PBF, V, CorrectedTauArray(i))

TotSepArray(i) = sep * FRRArray(i)

TotOtherArray(i) = Other * FRRArray(i) 'other

umPPCArray(i) = (FC + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) / (1 - inocticot) 'other

Worksheets("Storage").Cells(i + 1, 17).Value = umArray(i)

Worksheets("Storage").Cells(i + 1, 18).Value = umPPCArray(i)

'separation costs

TotSepArray(i) = sepArray(i) * FRR

sepPPCArray(i) = (FC + FRR + TotSepArray(i) + TotOther) / (1 - inocticot) 'other

```
Worksheets("Storage").Cells(i + 1, 19).Value = sepArray(i)
Worksheets("Storage").Cells(i + 1, 20).Value = sepPPCArray(i)
```

```
'other costs
```

```
TotOtherArray(i) = OtherArray(i) * FRR
```

```
OtherPPCArray(i) = (FC + FRR + TotSep + TotOtherArray(i)) / (1 - inoctot) 'other
```

```
Worksheets("Storage").Cells(i + 1, 21).Value = OtherArray(i)
```

```
Worksheets("Storage").Cells(i + 1, 22).Value = OtherPPCArray(i)
```

```
Next i
```

```
'Add titles to columns
```

```
Worksheets("Storage").Cells(1, 1).Value = "Glucose Cost"
```

```
Worksheets("Storage").Cells(1, 2).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 3).Value = "fpx"
```

```
Worksheets("Storage").Cells(1, 4).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 5).Value = "Yield"
```

```
Worksheets("Storage").Cells(1, 6).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 7).Value = "Interest Rate"
```

```
Worksheets("Storage").Cells(1, 8).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 9).Value = "Reactor Life"
```

```
Worksheets("Storage").Cells(1, 10).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 11).Value = "Half-velocity constant"
```

```
Worksheets("Storage").Cells(1, 12).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 13).Value = "So"
```

```
Worksheets("Storage").Cells(1, 14).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 15).Value = "Xo"
```

```
Worksheets("Storage").Cells(1, 16).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 17).Value = "Max Specific Growth Rate"
```

```
Worksheets("Storage").Cells(1, 18).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 19).Value = "Separation Percent"
```

```
Worksheets("Storage").Cells(1, 20).Value = "PPC"
```

```
Worksheets("Storage").Cells(1, 21).Value = "Other"
```

```
Worksheets("Storage").Cells(1, 22).Value = "PPC"
```

```
'complete sensitivity analysis and output results to Inputs Tab
```

```
Call Sensitivity(GArray(), GPPCArray(), 8, 5)
```

```
Call Sensitivity(PBFArray(), PBFPPCArray(), 9, 5)
```

```
Call Sensitivity(YArray(), YPPCArray(), 10, 5)
```

```
Call Sensitivity(IRArray(), IRPPCArray(), 14, 5)
```

```
Call Sensitivity(RLArray(), RLPPCArray(), 15, 5)
```

```
Call Sensitivity(ksArray(), ksPPCArray(), 17, 5)
```

```
Call Sensitivity(SoArray(), SoPPCArray(), 18, 5)
```

```
Call Sensitivity(XoArray(), XoPPCArray(), 19, 5)
```

```
Call Sensitivity(umArray(), umPPCArray(), 20, 5)
```

```
Call Sensitivity(sepArray(), sepPPCArray(), 23, 5)
```

Call Sensitivity(OtherArray(), OtherPPCArray(), 27, 5)

Worksheets("Results").Activate

LabelEndCode:

'-----Chart Code-----'

'=====

=====

'This code is designed to adjust the charts so that the y-axes all have the same ranges

Call GraphAdjustment("Chart 8", 1)
 Call GraphAdjustment("Chart 9", 3)
 Call GraphAdjustment("Chart 10", 5)
 Call GraphAdjustment("Chart 11", 7)
 Call GraphAdjustment("Chart 12", 9)
 Call GraphAdjustment("Chart 13", 11)
 Call GraphAdjustment("Chart 14", 13)
 Call GraphAdjustment("Chart 15", 15)
 Call GraphAdjustment("Chart 16", 17)
 Call GraphAdjustment("Chart 17", 19)
 Call GraphAdjustment("Chart 18", 21)

End Sub

Public Function FeedstockCost(ByVal Glucose As Double, ByVal ProductInBiomass As Double, ByVal Yield As Double) As Double

'Function Description: This function calculates the feedstock cost for glucose in terms of the final product in kg

FeedstockCost = Glucose / (ProductInBiomass * Yield)

End Function

Public Function ReactorCost(ByVal Volume As Double, ByVal intrate As Double, ByVal life As Double) As Double

'Function Description: This function uses principles discussed in Brown's book to calculate the ammortized capital cost

'for a reactor based on a volume supplied by the user and scale factors and multipliers available for reactors in the book

'based on data from Brown's book the scale factor and multiplier were found

SF = 0.71 'from Brown book for vertical process vessel

M = 7273 'used vertical process vessel with M of 6000 in 2002 dollars and converted to 2010 dollars

'Using economies of scale the capital cost can be calculated

$C_p = M * (\text{Volume} \wedge \text{SF})$

'Then using materials and labor values from Brown (Biorenewable Resources Book),
the grassroots capital is calculated

$$\text{MMF} = 1.04$$

$$\text{LMF} = 0.49$$

'Materials for installation

$$\text{CM} = \text{MMF} * \text{Cp}$$

'Direct labor

$$\text{CL} = \text{LMF} * (\text{Cp} + \text{CM})$$

'Direct capital cost

$$\text{CD} = \text{Cp} + \text{CM} + \text{CL}$$

'Indirect project Costs

'freight

$$\text{CFIT} = 0.08 * \text{Cp}$$

'Construction overhead

$$\text{CO} = 0.7 * \text{CL}$$

'engineering

$$\text{CE} = 0.15 * (\text{Cp} + \text{CM})$$

$$\text{CID} = \text{CFIT} + \text{CO} + \text{CE}$$

'Bare Module Cost

$$\text{CBM} = \text{CD} + \text{CID}$$

'contingency

$$\text{CCF} = 0.18 * \text{CBM}$$

'total module cost

$$\text{CTM} = \text{CBM} + \text{CCF}$$

'Auxiliary facilities

$$\text{CAF} = 0.3 * \text{CTM}$$

'Grassroots Capital

$$\text{CGR} = \text{CTM} + \text{CAF}$$

'output CGR to intermediate calculations page

If Worksheets("Intermediate Calculations").Range("E10").Value = 0 Then

Worksheets("Intermediate Calculations").Range("E10").Value = CGR

End If

'The PMT function in excel can be used to calculate the amortized value

ReactorCost = Abs(Application.WorksheetFunction.Pmt(intrate, life, CGR))

End Function

Public Function FermentorRRate(ByVal RC As Double, ByVal Titer As Double, ByVal
ProductInBiomass As Double, ByVal Volume As Double, ByVal RetentionTime As
Double) As Double

'Function Description: This function outputs the fermenter rate cost which

'FRR here doesn't account for inoculum

If Worksheets("Intermediate Calculations").Range("E22").Value = 0 Then

```

Worksheets("Intermediate Calculations").Range("E22").Value = Titer *
ProductInBiomass * Volume * (1 /
RetentionTime)
Worksheets("Intermediate Calculations").Range("G23").Value = Titer *
ProductInBiomass * Volume * (1 /
RetentionTime) * 24 * 350
End If

```

```

FermentorRRate = RC / ((Titer * ProductInBiomass * Volume * (1 / RetentionTime))
* 24 * 350)
End Function

```

```

Public Sub Simulation(ByRef SimArray() As Double, ByVal Value, ByVal uncertainty)
'Subroutine Description: This subroutine takes in an empty array, the initial value for
a given variable and its uncertainty and
'outputs an array with 100 values that go from the lower to upper bounds based on the
uncertainty
Dim NumValues As Integer, Up As Double, Low As Double
NumValues = 100
Up = Value * (1 + uncertainty)
Low = Value * (1 - uncertainty)

'create an array for 100 values that can be used to run simulations
StepSize = (Up - Low) / NumValues
B = 1
For A = Low To Up Step StepSize
SimArray(B) = A
B = B + 1
Next A
End Sub

```

```

Public Sub Sensitivity(ByRef InArray() As Double, OutArray() As Double, Row As
Integer, Column As Integer)
'This subroutine completes the sensitivity analysis and outputs the results in the
designated row and column of the inputs tab
'Red values are negative and green values are positive

Dim PercentChangeIn As Double, PercentChangeOut As Double, Slope As Double

PercentChangeIn = (InArray(50) - InArray(49)) / InArray(50)
PercentChangeOut = (OutArray(50) - OutArray(49)) / OutArray(50)
Slope = PercentChangeOut / PercentChangeIn
Worksheets("Inputs").Cells(Row, Column).Value = Slope

If Slope > 0 Then
Worksheets("Inputs").Cells(Row, Column).Interior.Color = RGB(51, 153,
102) 'green

```

```

Else
Worksheets("Inputs").Cells(Row, Column).Interior.Color = RGB(128, 0, 0)
'red
End If
End Sub

Public Sub GraphAdjustment(ChartNum As String, ColRef As Integer)
'This subroutine is designed to adjust the graphs for L1 L2 and L3 analyses
ActiveSheet.ChartObjects(ChartNum).Activate
ActiveSheet.ChartObjects(ChartNum).Chart.Axes(xlValue).MaximumScale =
Worksheets("Storage").Range("B107").Value
ActiveSheet.ChartObjects(ChartNum).Chart.Axes(xlValue).MinimumScale =
Worksheets("Storage").Range("B106").Value

With ActiveChart.Axes(xlCategory, xlPrimary)
.MaximumScale = Worksheets("Storage").Cells(104, ColRef)
.MinimumScale = Worksheets("Storage").Cells(103, ColRef)
End With
End Sub

Public Function LogisticEq(ByRef HalfVelocity As Double, Yield As Double, SubstrateC
As Double, CellC As Double, MaxSGR As Double) As Double
'function description; this function outputs the fermenter reaction time based on a
kinetic model described in Shuler and Kargi
Dim A As Double, B As Double, Term1 As Double, Term2 As Double, Xfinal As
Double

A = HalfVelocity * Yield
B = SubstrateC * Yield
Xfinal = 0.95 * (B + CellC)
Term1 = ((A + B + CellC) / (B + CellC)) *
Application.WorksheetFunction.Ln(Xfinal / CellC)
Term2 = (A / (B + CellC)) * Application.WorksheetFunction.Ln((B + CellC +
Xfinal) / B)
LogisticEq = (Term1 - Term2) / MaxSGR
End Function

```

Level 2 Analysis

Level 2 Description

In cases where not all of the kinetic parameters are available for an experiment, a simpler analysis was developed to allow insight into the economics of industrial fermentation (termed Level 2 Analysis). While the Level 2 (L2) analysis incorporates some kinetic variables, it does not compute the fermentation time using the Logistic Equation. For example, X_f , τ , and the inoculum required are inputs for the model rather than intermediate calculations. Figures 4A, 5A, and 6A illustrate the interface, intermediate calculations, and results page for the L2 analysis. While figure 6A does not show the all of the graphs generated by a L2 analysis it is provided to show a magnified view of the results page in figure 3A.

	A	B	C	D	E	F
1						
2		Run L2 Analysis				
3						
4						
5	Inputs					
6						
7	<i>Feedstock Cost Inputs</i>	Reference Values	Testing Values	Uncertainty (%)	Sensitivity Coefficient	Units
8	Glucose Cost	\$0.12	\$0.45	5%	0.541	\$/kg glucose
9	f_{pk}	0.80	0.80	10%	-1.002	
10	Y_{xs}	0.50	0.62	10%	-0.543	
11						
12	<i>Fermenter Rental Rate Inputs</i>					
13	Fermenter Volume, V	500	100			cubic meters
14	Interest Rate	15%	15.0%	10%	0.261	per year
15	Reactor Life	10	10	10%	-0.211	years
16	X_f	33.75	67.8	10%	-0.460	
17	τ	500.0	67.0	10%	0.337	
18	Downtime between Runs		24.0	10%	0.121	
19	Inoculum Required		10.0%	10%	0.111	% of reactor volume
20						
21	<i>Other Costs</i>					
22	Separation Cost		40%	10%	0.114	
23	Other Costs		20%	10%	0.057	
24	Target Product Price		\$5.00			
25						

Figure 4A. 2L Inputs Page.

Intermediate Calculations: Only calculated values for the given level of analysis are shown here.

Glucose Cost f_{px} Y_{xs}	}	Feedstock Cost, \$/kg prod.	\$0.91
<hr/>			
Volume Multiplier Scale Factor	}	Interest Rate Reactor Cost Reactor Life	\$1,210,589
		Amortized Capital Cost	\$241,212
<hr/>			
K_s S_o X_o μ_m	}	τ , hrs Downtime between loading	}
		Corrected τ	
<hr/>			
Corrected τ X_f f_{px} Fermenter Volume, V Reactor Cost	}	Production Rate, kg/hr Hours per year	59.6
		Annual Production Rate, kg/yr	500,677
<hr/>			
X_f τ f_{px}	}	Productivity, g/L-hr	0.81
<hr/>			
X_f Corrected τ f_{px}	}	Productivity, g/L-hr	0.60
<hr/>			

Figure 5A. L2 Intermediate Calculations Page.

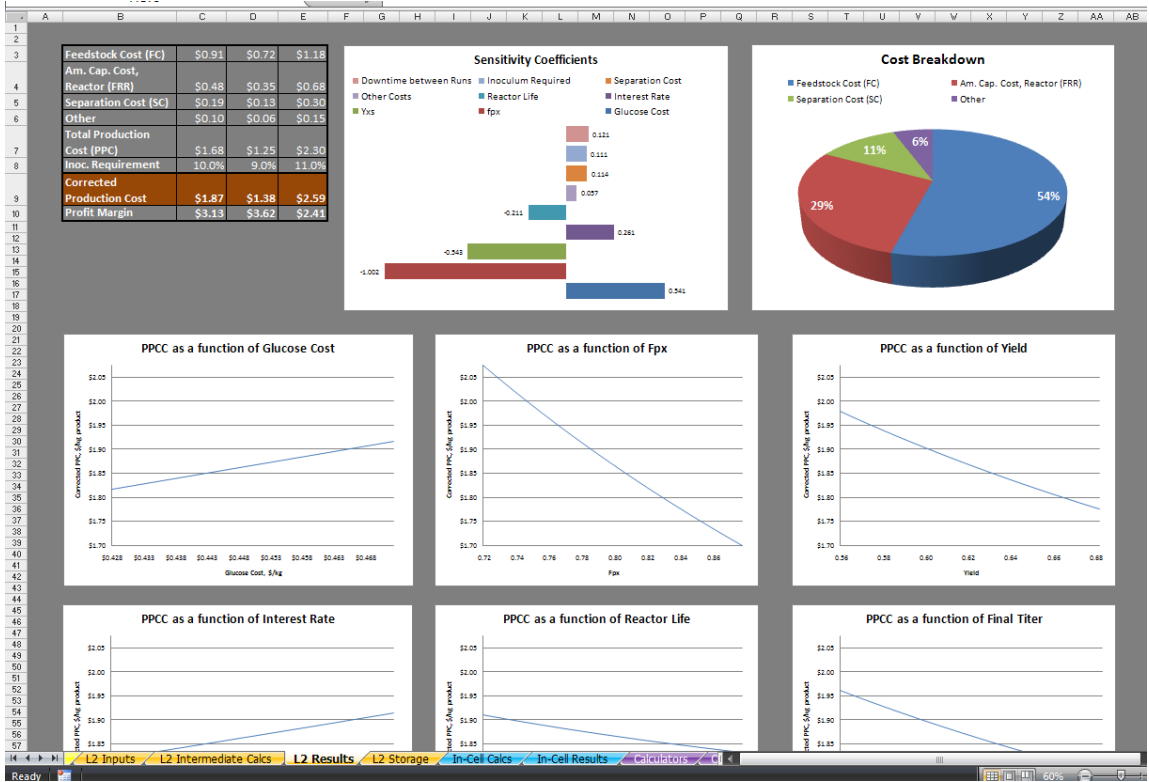


Figure 6A. L2 Results Page.

L2 Code

```
Private Sub CommandButton1_Click()
```

```
'Program Description: This program computes the corrected product production cost for a
given compound of interest using glucose as the feedstock.
```

```
'This is a level 2 analysis that does not include kinetic variables.
```

```
'Program Author: Carol Faulhaber
```

```
'Date: 2/7/11
```

```
'Dimension variables
```

```
Dim GArray(1000) As Double, G As Double, GU As Double, Gbest As Double, Gworst
As Double
```

```
Dim PBFArray(1000) As Double, PBF As Double, PBFU As Double, PBFbest As Double,
PBFworst As Double
```

```
Dim YArray(1000) As Double, Y As Double, YU As Double, Ybest As Double, Yworst
As Double
```

```
Dim FC As Double, FCbest As Double, FCworst As Double, FCSim As Double
```

```
Dim V As Double, VU As Double
```

```
Dim IR As Double, IRU As Double, IRBest As Double, IRWorst As Double,
IRArray(1000) As Double
```

```
Dim RL As Double, RLU As Double, RLbest As Double, RLworst As Double,
RLArray(1000) As Double
```

```
Dim Xf As Double, XfU As Double, XfBest As Double, XfWorst As Double,
XfArray(1000) As Double
```

```
Dim Tau As Double, TauU As Double, TauBest As Double, TauWorst As Double,
TauArray(1000) As Double
```

```
Dim RC As Double, RCbest As Double, RCworst As Double
```

```
Dim FRR As Double, FRRBest As Double, FRRWorst As Double
```

```
Dim sep As Double, sepU As Double, sepArray(1000) As Double
```

```
Dim inoc As Double, inocU As Double, inocArray(1000) As Double
```

```
Dim Downtime As Double, DowntimeU As Double, DowntimeArray(1000) As Double
```

```
Dim Other As Double, OtherU As Double, OtherArray(1000) As Double
```

```
Dim Productivity As Double
```

```
Dim GPPCArray(1000) As Double, PBFPPCArray(1000) As Double, YPPCArray(1000)
As Double, IRPPCArray(1000) As Double, RLPPCArray(1000) As Double
```

```
Dim XfPPCArray(1000) As Double, TauPPCArray(1000) As Double, RCPPCArray(1000)
As Double, SoPPCArray(1000) As Double, XoPPCArray(1000) As Double
```

```
Dim ksPPCArray(1000) As Double, umPPCArray(1000) As Double, sepPPCArray(100)
As Double
```

```
Dim FCArray(1000) As Double, FRRArray(1000) As Double, TotSepArray(1000) As
Double, RCArray(1000) As Double
```

```
Dim CorrectedTauArray(1000) As Double, ksArray(1000) As Double, inocTotArray(1000)
As Double
```

```
Dim OtherPPCArray(1000) As Double, TotOtherArray(1000) As Double
```

```
Dim DTPPCArray(1000) As Double, inocPPCArray(1000) As Double
```



```

=====
'-----Level 2 calculations-----
Level2Calculations:

'Read in variables
G = Worksheets("L2 Inputs").Range("C8").Value 'glucose cost
GU = Worksheets("L2 Inputs").Range("D8").Value 'uncertainty in glucose cost
PBF = Worksheets("L2 Inputs").Range("C9").Value 'product in biomass
PBFU = Worksheets("L2 Inputs").Range("D9").Value 'uncertainty in product in biomass
Y = Worksheets("L2 Inputs").Range("C10").Value 'yield
YU = Worksheets("L2 Inputs").Range("D10").Value 'yield uncertainty
V = Worksheets("L2 Inputs").Range("C13").Value 'reactor volume
IR = Worksheets("L2 Inputs").Range("C14").Value 'interest rate
IRU = Worksheets("L2 Inputs").Range("D14").Value 'interest rate uncertainty
RL = Worksheets("L2 Inputs").Range("C15").Value 'reactor life
RLU = Worksheets("L2 Inputs").Range("D15").Value 'reactor life uncertainty
Xf = Worksheets("L2 Inputs").Range("C16").Value
XfU = Worksheets("L2 Inputs").Range("D16").Value
Tau = Worksheets("L2 Inputs").Range("C17").Value 'retention time for fermentation
TauU = Worksheets("L2 Inputs").Range("D17").Value 'uncertainty in retention time
Downtime = Worksheets("L2 Inputs").Range("C18").Value 'downtime between loadings
DowntimeU = Worksheets("L2 Inputs").Range("D18").Value 'downtime between loadings
uncertainty
inoc = Worksheets("L2 Inputs").Range("C19").Value 'inoculum required
inocU = Worksheets("L2 Inputs").Range("D19").Value 'inoculum required
sep = Worksheets("L2 Inputs").Range("C22").Value 'separation costs
sepU = Worksheets("L2 Inputs").Range("D22").Value 'sep cost uncertainty
Other = Worksheets("L2 Inputs").Range("C23").Value 'other costs
OtherU = Worksheets("L2 Inputs").Range("D23").Value 'other cost uncertainty

'-----Complete FC Calculations. For L2 analysis PPC=FC+FR+SC-----
-----
'Calculations that output to inputs tab
CorrectedTau = Tau + Downtime
Worksheets("L2 Intermediate Calcs").Range("G16").Value = CorrectedTau
Productivity = PBF * (Xf / Tau)
ProductivityCorrected = PBF * (Xf / CorrectedTau)
Worksheets("L2 Intermediate Calcs").Range("E28").Value = Productivity
Worksheets("L2 Intermediate Calcs").Range("E42").Value = ProductivityCorrected

'Basecase Calculations

```

$FC = \text{FeedstockCost}(G, PBF, Y)$
 $\text{Worksheets}("L2 \text{ Intermediate Calcs"}).Range("E5").Value = FC$
 $RC = \text{ReactorCost}(V, IR, RL)$
 $\text{Worksheets}("L2 \text{ Intermediate Calcs"}).Range("H10").Value = RC$
 'Capital Reactor cost inserted into intermediate calculations within function (total)
 $FRR = \text{FermentorRRate}(RC, Xf, PBF, V, \text{CorrectedTau})$
 $\text{TotSep} = \text{sep} * FRR$
 $\text{TotOther} = \text{Other} * FRR$

'WorstCase Calculations

$G_{\text{worst}} = G * (1 + GU)$
 $PBF_{\text{worst}} = PBF * (1 - PBFU)$
 $Y_{\text{worst}} = Y * (1 - YU)$
 $FC_{\text{worst}} = \text{FeedstockCost}(G_{\text{worst}}, PBF_{\text{worst}}, Y_{\text{worst}})$
 $IR_{\text{worst}} = IR * (1 + IRU)$
 $RL_{\text{worst}} = RL * (1 - RLU)$
 $RC_{\text{worst}} = \text{ReactorCost}(V, IR_{\text{worst}}, RL_{\text{worst}})$
 $Xf_{\text{worst}} = Xf * (1 - XfU)$
 $\text{Downtime}_{\text{worst}} = \text{Downtime} * (1 + \text{DowntimeU})$
 $\text{CorrectedTau}_{\text{worst}} = \text{Tau} + \text{Downtime}_{\text{worst}}$
 $FRR_{\text{worst}} = \text{FermentorRRate}(RC_{\text{worst}}, Xf_{\text{worst}}, PBF_{\text{worst}}, V, \text{CorrectedTau}_{\text{worst}})$
 $\text{Sep}_{\text{worst}} = \text{sep} * (1 + \text{sepU})$
 $\text{TotSep}_{\text{worst}} = \text{Sep}_{\text{worst}} * FRR_{\text{worst}}$
 $\text{Other}_{\text{worst}} = \text{Other} * (1 + \text{OtherU})$
 $\text{TotOther}_{\text{worst}} = \text{Other}_{\text{worst}} * FRR_{\text{worst}}$
 $\text{inoc}_{\text{worst}} = \text{inoc} * (1 + \text{inocU})$

'BestCase Calculations

$G_{\text{best}} = G * (1 - GU)$
 $PBF_{\text{best}} = PBF * (1 + PBFU)$
 $Y_{\text{best}} = Y * (1 + YU)$
 $FC_{\text{best}} = \text{FeedstockCost}(G_{\text{best}}, PBF_{\text{best}}, Y_{\text{best}})$
 $IR_{\text{best}} = IR * (1 - IRU)$
 $RL_{\text{best}} = RL * (1 + RLU)$
 $RC_{\text{best}} = \text{ReactorCost}(V, IR_{\text{best}}, RL_{\text{best}})$
 $Xf_{\text{best}} = Xf * (1 + XfU)$
 $\text{Downtime}_{\text{best}} = \text{Downtime} * (1 - \text{DowntimeU})$
 $\text{CorrectedTau}_{\text{best}} = \text{Tau} + \text{Downtime}_{\text{best}}$
 $FRR_{\text{best}} = \text{FermentorRRate}(RC_{\text{best}}, Xf_{\text{best}}, PBF_{\text{best}}, V, \text{CorrectedTau}_{\text{best}})$
 $\text{Sep}_{\text{best}} = \text{sep} * (1 - \text{sepU})$
 $\text{TotSep}_{\text{best}} = \text{Sep}_{\text{best}} * FRR_{\text{best}}$
 $\text{Other}_{\text{best}} = \text{Other} * (1 - \text{OtherU})$
 $\text{TotOther}_{\text{best}} = \text{Other}_{\text{best}} * FRR_{\text{best}}$
 $\text{inoc}_{\text{best}} = \text{inoc} * (1 - \text{inocU})$

```
'Output baseline, best and worst case scenarios
Worksheets("L2 Results").Range("C3").Value = FC
Worksheets("L2 Results").Range("D3").Value = FCbest
Worksheets("L2 Results").Range("E3").Value = FCworst
Worksheets("L2 Results").Range("C4").Value = FRR
Worksheets("L2 Results").Range("D4").Value = FRRBest
Worksheets("L2 Results").Range("E4").Value = FRRWorst
Worksheets("L2 Results").Range("C5").Value = TotSep
Worksheets("L2 Results").Range("D5").Value = TotSepBest
Worksheets("L2 Results").Range("E5").Value = TotSepWorst
Worksheets("L2 Results").Range("C6").Value = TotOther
Worksheets("L2 Results").Range("D6").Value = TotOtherBest
Worksheets("L2 Results").Range("E6").Value = TotOtherWorst
Worksheets("L2 Results").Range("C8").Value = inoc
Worksheets("L2 Results").Range("D8").Value = inocBest
Worksheets("L2 Results").Range("E8").Value = inocWorst
```

```
'-----Begin Simulations-----
```

```
-----
'Assign Arrays for each input. Each array will contain 100 values and is based on the
uncertainty
```

```
Call Simulation(GArray(), G, GU)
Call Simulation(PBFArray(), PBF, PBFU)
Call Simulation(YArray(), Y, YU)
Call Simulation(IRArray(), IR, IRU)
Call Simulation(RLArray(), RL, RLU)
Call Simulation(XfArray(), Xf, XfU)
Call Simulation(TauArray(), Tau, TauU)
Call Simulation(sepArray(), sep, sepU)
Call Simulation(OtherArray(), Other, OtherU)
Call Simulation(DowntimeArray(), Downtime, DowntimeU)
Call Simulation(inocArray(), inoc, inocU)
```

```
'Loop through all data and output results to storage tab
For i = 1 To 100
```

```
  'glucose cost
  FCArray(i) = FeedstockCost(GArray(i), PBF, Y)
  GPPCArray(i) = (FCArray(i) + FRR + TotSep + TotOther) / (1 - inoc)
  Worksheets("L2 Storage").Cells(i + 1, 1).Value = GArray(i)
  Worksheets("L2 Storage").Cells(i + 1, 2).Value = GPPCArray(i)
```

```
  'fraction of biomass in product
  FCArray(i) = FeedstockCost(G, PBFArray(i), Y)
  FRRArray(i) = FermentorRRate(RC, Xf, PBFArray(i), V, CorrectedTau)
  TotSepArray(i) = sep * FRRArray(i)
```

TotOtherArray(i) = Other * FRRArray(i)
 PBFPPCArray(i) = (FCArray(i) + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) /
 (1 - inoc)

Worksheets("L2 Storage").Cells(i + 1, 3).Value = PBFArray(i)
 Worksheets("L2 Storage").Cells(i + 1, 4).Value = PBFPPCArray(i)

'Yield

FCArray(i) = FeedstockCost(G, PBF, YArray(i))
 YPPCArray(i) = (FCArray(i) + FRR + TotSep + TotOther) / (1 - inoc)
 Worksheets("L2 Storage").Cells(i + 1, 5).Value = YArray(i)
 Worksheets("L2 Storage").Cells(i + 1, 6).Value = YPPCArray(i)

'Interest Rate

RCArray(i) = ReactorCost(V, IRArray(i), RL)
 FRRArray(i) = FermentorRRate(RCArray(i), Xf, PBF, V, CorrectedTau)
 TotSepArray(i) = sep * FRRArray(i)
 TotOtherArray(i) = Other * FRRArray(i)
 IRPPCArray(i) = (FC + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) / (1 - inoc)
 Worksheets("L2 Storage").Cells(i + 1, 7).Value = IRArray(i)
 Worksheets("L2 Storage").Cells(i + 1, 8).Value = IRPPCArray(i)

'Reactor Life

RCArray(i) = ReactorCost(V, IR, RLArray(i))
 FRRArray(i) = FermentorRRate(RCArray(i), Xf, PBF, V, CorrectedTau)
 TotSepArray(i) = sep * FRRArray(i)
 TotOtherArray(i) = Other * FRRArray(i)
 RLPPCArray(i) = (FC + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) / (1 - inoc)
 Worksheets("L2 Storage").Cells(i + 1, 9).Value = RLArray(i)
 Worksheets("L2 Storage").Cells(i + 1, 10).Value = RLPPCArray(i)

'Titer

FRRArray(i) = FermentorRRate(RC, XfArray(i), PBF, V, CorrectedTau)
 TotSepArray(i) = sep * FRRArray(i)
 TotOtherArray(i) = Other * FRRArray(i)
 XfPPCArray(i) = (FC + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) / (1 - inoc)
 Worksheets("L2 Storage").Cells(i + 1, 11).Value = XfArray(i)
 Worksheets("L2 Storage").Cells(i + 1, 12).Value = XfPPCArray(i)

'Tau

CorrectedTauArray(i) = TauArray(i) + Downtime
 FRRArray(i) = FermentorRRate(RC, Xf, PBF, V, CorrectedTauArray(i))
 TotSepArray(i) = sep * FRRArray(i)
 TotOtherArray(i) = Other * FRRArray(i)
 TauPPCArray(i) = (FC + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) / (1 - inoc)
 Worksheets("L2 Storage").Cells(i + 1, 13).Value = TauArray(i)
 Worksheets("L2 Storage").Cells(i + 1, 14).Value = TauPPCArray(i)

'separation costs

TotSepArray(i) = sepArray(i) * FRR

sepPPCArray(i) = (FC + FRR + TotSepArray(i) + TotOther) / (1 - inoc)

Worksheets("L2 Storage").Cells(i + 1, 15).Value = sepArray(i)

Worksheets("L2 Storage").Cells(i + 1, 16).Value = sepPPCArray(i)

'Other costs

TotOtherArray(i) = OtherArray(i) * FRR

OtherPPCArray(i) = (FC + FRR + TotSep + TotOtherArray(i)) / (1 - inoc)

Worksheets("L2 Storage").Cells(i + 1, 17).Value = OtherArray(i)

Worksheets("L2 Storage").Cells(i + 1, 18).Value = OtherPPCArray(i)

'Downtime

CorrectedTauArray(i) = Tau + DowntimeArray(i)

FRRArray(i) = FermentorRRate(RC, Xf, PBF, V, CorrectedTauArray(i))

TotSepArray(i) = sep * FRRArray(i)

TotOtherArray(i) = Other * FRRArray(i)

DTPPCArray(i) = (FC + FRRArray(i) + TotSepArray(i) + TotOtherArray(i)) / (1 - inoc)

Worksheets("L2 Storage").Cells(i + 1, 19).Value = DowntimeArray(i)

Worksheets("L2 Storage").Cells(i + 1, 20).Value = DTPPCArray(i)

'inoculum

inocPPCArray(i) = (FC + FRR + TotSep + TotOther) / (1 - inocArray(i))

Worksheets("L2 Storage").Cells(i + 1, 21).Value = inocArray(i)

Worksheets("L2 Storage").Cells(i + 1, 22).Value = inocPPCArray(i)

Next i

'Add titles to columns

Worksheets("L2 Storage").Cells(1, 1).Value = "Glucose Cost"

Worksheets("L2 Storage").Cells(1, 2).Value = "PPC"

Worksheets("L2 Storage").Cells(1, 3).Value = "fpx"

Worksheets("L2 Storage").Cells(1, 4).Value = "PPC"

Worksheets("L2 Storage").Cells(1, 5).Value = "Yield"

Worksheets("L2 Storage").Cells(1, 6).Value = "PPC"

Worksheets("L2 Storage").Cells(1, 7).Value = "Interest Rate"

Worksheets("L2 Storage").Cells(1, 8).Value = "PPC"

Worksheets("L2 Storage").Cells(1, 9).Value = "Reactor Life"

Worksheets("L2 Storage").Cells(1, 10).Value = "PPC"

Worksheets("L2 Storage").Cells(1, 11).Value = "Titer"

Worksheets("L2 Storage").Cells(1, 12).Value = "PPC"

Worksheets("L2 Storage").Cells(1, 13).Value = "Tau"

Worksheets("L2 Storage").Cells(1, 14).Value = "PPC"

Worksheets("L2 Storage").Cells(1, 15).Value = "Separation Percent"

Worksheets("L2 Storage").Cells(1, 16).Value = "PPC"

```
Worksheets("L2 Storage").Cells(1, 17).Value = "Other"
Worksheets("L2 Storage").Cells(1, 18).Value = "PPC"
Worksheets("L2 Storage").Cells(1, 19).Value = "Downtime"
Worksheets("L2 Storage").Cells(1, 20).Value = "PPC"
Worksheets("L2 storage").Cells(1, 21).Value = "inoculum"
Worksheets("L2 storage").Cells(1, 22).Value = "PPC"
```

```
'complete sensitivity analysis and output results to Inputs Tab
```

```
Call Sensitivity(GArray(), GPPCArray(), 8, 5)
Call Sensitivity(PBFArray(), PBFPPCArray(), 9, 5)
Call Sensitivity(YArray(), YPPCArray(), 10, 5)
Call Sensitivity(IRArray(), IRPPCArray(), 14, 5)
Call Sensitivity(RLArray(), RLPPCArray(), 15, 5)
Call Sensitivity(XfArray(), XfPPCArray(), 16, 5)
Call Sensitivity(TauArray(), TauPPCArray(), 17, 5)
Call Sensitivity(sepArray(), sepPPCArray(), 22, 5)
Call Sensitivity(OtherArray(), OtherPPCArray(), 23, 5)
Call Sensitivity(DowntimeArray(), DTPPCArray(), 18, 5)
Call Sensitivity(inocArray(), inocPPCArray(), 19, 5)
```

```
Worksheets("L2 Results").Activate
```

```
Call GraphAdjustment("Chart 3", 1)
Call GraphAdjustment("Chart 7", 3)
Call GraphAdjustment("Chart 8", 5)
Call GraphAdjustment("Chart 9", 7)
Call GraphAdjustment("Chart 10", 9)
Call GraphAdjustment("Chart 11", 11)
Call GraphAdjustment("Chart 12", 13)
Call GraphAdjustment("Chart 13", 15)
Call GraphAdjustment("Chart 14", 17)
Call GraphAdjustment("Chart 15", 19)
Call GraphAdjustment("Chart 16", 21)
```

```
End Sub
```

```
Public Function FeedstockCost(ByVal Glucose As Double, ByVal ProductInBiomass As
Double, ByVal Yield As Double) As Double
```

```
'Function Description: This function calculates the feedstock cost for glucose in terms
of the final product in kg
```

```
FeedstockCost = Glucose / (ProductInBiomass * Yield)
End Function
```

Public Function ReactorCost(ByVal Volume As Double, ByVal intrate As Double, ByVal life As Double) As Double

'Function Description: This function uses principles discussed in Brown's book to calculate the ammortized capital cost

'for a reactor based on a volume supplied by the user and scale factors and multipliers available for reactors in the book

'based on data from Brown's book the scale factor and multiplier were found

SF = 0.71 'from Brown book for vertical process vessel

M = 7273 'used vertical process vessel with M of 6000 in 2002 dollars and converted to 2010 dollars

'Using economies of scale the capital cost can be calculated

$C_p = M * (\text{Volume} \wedge \text{SF})$

'Then using materials and labor values from Brown (Biorenewable Resources Book), the grassroots capital is calculated

MMF = 1.04

LMF = 0.49

'Materials for installation

$CM = MMF * C_p$

'Direct labor

$CL = LMF * (C_p + CM)$

'Direct capital cost

$CD = C_p + CM + CL$

'Indirect project Costs

'freight

$CFIT = 0.08 * C_p$

'Construction overhead

$CO = 0.7 * CL$

'engineering

$CE = 0.15 * (C_p + CM)$

$CID = CFIT + CO + CE$

'Bare Module Cost

$CBM = CD + CID$

'contingency

$CCF = 0.18 * CBM$

'total module cost

$CTM = CBM + CCF$

'Auxiliary facilities

$CAF = 0.3 * CTM$

'Grassroots Capital

$CGR = CTM + CAF$

'output CGR to intermediate calculations page

If Worksheets("L2 Intermediate Calcs").Range("E10").Value = 0 Then

Worksheets("L2 Intermediate Calcs").Range("E10").Value = CGR

End If

The PMT function in excel can be used to calculate the amortized value
 $\text{ReactorCost} = \text{Abs}(\text{Application.WorksheetFunction.Pmt}(\text{intrate}, \text{life}, \text{CGR}))$

End Function

Public Function FermentorRRate(ByVal RC As Double, ByVal Titer As Double, ByVal ProductInBiomass As Double, ByVal Volume As Double, ByVal RetentionTime As Double) As Double

'Function Description: This function outputs the fermenter rate cost which
 'FRR here doesn't account for inoculum

If Worksheets("L2 Intermediate Calcs").Range("E22").Value = 0 Then
 Worksheets("L2 Intermediate Calcs").Range("E22").Value = Titer *
 ProductInBiomass * Volume * (1 / RetentionTime)
 Worksheets("L2 Intermediate Calcs").Range("G23").Value = Titer *
 ProductInBiomass * Volume * (1 / RetentionTime) * 24 *
 350

End If

FermentorRRate = RC / ((Titer * ProductInBiomass * Volume * (1 / RetentionTime))
 * 24 * 350)

End Function

Public Sub Simulation(ByRef SimArray() As Double, ByVal Value, ByVal uncertainty)

'Subroutine Description: This subroutine takes in an empty array, the initial value for
 a given variable and its uncertainty and

'outputs an array with 100 values that go from the lower to upper bounds based on the
 uncertainty

Dim NumValues As Integer, Up As Double, Low As Double

NumValues = 100

Up = Value * (1 + uncertainty)

Low = Value * (1 - uncertainty)

'create an array for 100 values that can be used to run simulations

StepSize = (Up - Low) / NumValues

B = 1

For A = Low To Up Step StepSize

 SimArray(B) = A

 B = B + 1

Next A

End Sub

Public Sub Sensitivity(ByRef InArray() As Double, OutArray() As Double, Row As Integer, Column As Integer)

'This subroutine completes the sensitivity analysis and outputs the results in the designated row and column of the inputs tab

'Red values are negative and green values are positive

Dim PercentChangeIn As Double, PercentChangeOut As Double, Slope As Double

PercentChangeIn = (InArray(50) - InArray(49)) / InArray(50)

PercentChangeOut = (OutArray(50) - OutArray(49)) / OutArray(50)

Slope = PercentChangeOut / PercentChangeIn

Worksheets("L2 Inputs").Cells(Row, Column).Value = Slope

If Slope > 0 Then

Worksheets("L2 Inputs").Cells(Row, Column).Interior.Color = RGB(51, 153,
102) 'green

Else

Worksheets("L2 Inputs").Cells(Row, Column).Interior.Color = RGB(128, 0,
0) 'red

End If

End Sub

Public Sub GraphAdjustment(ChartNum As String, ColRef As Integer)

'This subroutine is designed to adjust the graphs for L1 L2 and L3 analyses

ActiveSheet.ChartObjects(ChartNum).Activate

ActiveSheet.ChartObjects(ChartNum).Chart.Axes(xlValue).MaximumScale =
Worksheets("L2 Storage").Range("B107").Value

ActiveSheet.ChartObjects(ChartNum).Chart.Axes(xlValue).MinimumScale =
Worksheets("L2 Storage").Range("B106").Value

With ActiveChart.Axes(xlCategory, xlPrimary)

.MaximumScale = Worksheets("L2 Storage").Cells(104, ColRef)

.MinimumScale = Worksheets("L2 Storage").Cells(103, ColRef)

End With

End Sub

Public Function LogisticEq(ByRef HalfVelocity As Double, Yield As Double, SubstrateC
As Double, CellC As Double, MaxSGR As Double) As Double

'function description; this function outputs the fermenter reaction time based on a
kinetic model described in Shuler and Kargi

Dim A As Double, B As Double, Term1 As Double, Term2 As Double, Xfinal As
Double

A = HalfVelocity * Yield

B = SubstrateC * Yield

Xfinal = 0.95 * (B + CellC)

Term1 = ((A + B + CellC) / (B + CellC)) *

Application.WorksheetFunction.Ln(Xfinal / CellC)

```
Term2 = (A / (B + CellC)) * Application.WorksheetFunction.Ln((B + CellC +  
Xfinal) / B)  
LogisticEq = (Term1 - Term2) / MaxSGR
```

```
End Function
```

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