

WORCESTER POLYTECHNIC INSTITUTE

Marketing Production and Financial Analysis of FDCA

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Abstract

The objective of this project was to examine the feasibility of the production of FDCA on an industrial scale and its profitability in the market. The rationale for this project was to identify alternative building blocks to replace fossil-based ones during manufacturing processes in the hopes of reducing the emission of CO₂ and create a greener environment. The methods used to complete this project include axiomatic design on the manufacturing objective, financial analysis and legal analysis on intellectual property. The results showed tremendous potential in the production of FDCA because its production method is feasible and profit could potentially be considerable. The conclusion also indicates that the analytic tools used in the process were effective throughout the decision making process and can be applied to solve real-world problems in the future.

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Chap. 1 -- Introduction

1.1 Problem Statement

In an effort to stay competitive in the pharmaceutical industry and align the company's mission with China's policies of "sustainable development", Qingquan medical and chemical is constantly seeking innovative methods to replace current methods in producing pharmaceutical intermediates. They have recently discovered a promising chemical product 2,5-furandicarboxylic acid (FDCA). Derived from fructose, 2,5-furandicarboxylic acid (FDCA) could be the key molecule in new plant-based plastics. 2,5-furandicarboxylic acid (FDCA) is a renewable, greener substitute for terephthalate in the production of polyesters, and it is commonly used as a precursor for the synthesis of bio-based polyesters and various other polymers (Sigma-Aldrich, 2018). Since 2,5-furandicarboxylic acid (FDCA) is still under experimental stage, the company is still assessing the possibility of mass-producing 2,5-furandicarboxylic acid (FDCA) and its profitability.

1.2 The Project Objective

The objective of this project is to examine the feasibility of production on an industrial scale of 2,5-furandicarboxylic acid (FDCA) and its profitability in the market. In order to accomplish this objective, the following objectives were accomplished:

- Preliminary market and product research including: 1) product value, 2) its manufacturing processes, 3) its potential in the secondary market. 4) future

competition in the market and their current development.

- Research legal implications in terms of ways to avoid intellectual property infringement.

- Create a financial analysis for possible future returns.

From these deliverables, an understanding of the potential of 2,5-furandicarboxylic acid (FDCA) from different perspectives and ultimately evaluated whether 2,5-furandicarboxylic acid (FDCA) should be mass-produced.

1.3 Rationale

Human beings might be on the way to deplete and over-consume natural resources. In the 21st century, the topic of sustainable development and green growth is being talked about at length. The majority of industries are researching for innovative procedures or substitutes to replace their current practice. Biomass is an abundant renewable carbon source for the sustainable supply of valuable intermediates for the production of fuels, chemicals, and bio-based plastics (Academic Press, 1998). 2,5-furandicarboxylic acid (FDCA) is a significant renewable building block due to its potential as a substitute for various petrochemical, such as terephthalic acid and adipic acid (Production of adipic acid and derivatives from carbohydrate-containing material, 2013). 2,5-furandicarboxylic acid (FDCA) has numerous potential applications that include polyesters, polyurethanes, and polyamides. In addition, a copolymer of ethylene glycol and FDCA, Polyethylene furanoate (PEF), has the ability to vastly improve the mechanical properties compared

to polyethylene terephthalate, such as higher glass transition temperature and improved tensile modulus. In addition, PEF has also shown better gas barrier properties for oxygen, which can ultimately be contributed to the production of water bottles, food packaging, sports apparel, and footwear. Accordingly, a strategic consortium of global companies is in the process of developing technology for the production of this bioplastic (Meet Our Partners: Plant PET Technology Collaborative, 2013). With PEF and other FDCA derivatives presenting such tremendous potential in the industry, Qingquan Medical & Chemical finds it imperative to develop an accessible and economical approach to produce FDCA.

1.4 State-of-the-Art

Major participants in the market including DuPont has announced the production of FDCA for use in PTF. In March 2016, Avantium, and BASF has also established a joint venture Synvina to set up a 50,000 t/a plant for the production of FDCA based on fructose at BASF's Verbund-site in Antwerp, Belgium. The inflow of a considerable amount of capitals indicates a tremendous potential and profitable outlook in the market of FDCA. However, considering the size of these companies, the fact that the production of FDCA has been limited to fairly small quantities also suggests that the details of the production still need to be figured out in terms of its economic production route, the yield and estimated cost on an industrial scale.

Chapter 2 -- Methods

This section provides a brief explanation of the procedures used to complete this project and its justifications for all of the procedures. The objective of the project is facilitated by developing an axiomatic design matrix with the intention of the production of 2,5-furandicarboxylic acid (FDCA) along with four relevant analyses, including 1) product and market research, 2) financial analysis, 3) legal analysis, 4) risk analysis, all of which will ultimately support the decision surrounding feasibility and profitability of producing 2,5-furandicarboxylic acid (FDCA). After providing the results of the findings, conclusions will be drawn.

The 5 analytic tools in the table below were used to complete this project.

Analytic Methods	Purpose
Axiomatic Design	Promote definition of each procedure in the production process
Product and Market Research	Identify the strength and weakness of FDCA and understand its potential in the market and secondary market, as well as future competition in the industry.
Financial Analysis	Determine the estimated capital investment and evaluate the net present value on a five-year plan.
Legal Analysis	Identify approaches to avoid intellectual property infringement.

Table 1: Methods

2.1 Axiomatic Design

Axiomatic design is dedicated to find the commonality of all good designs and attempts to develop a universal approach to all designing problems. By creating an axiomatic design focused on the production of FDCA, the customer needs are translated to functional requirements, which are then satisfied by their respective design parameters. In the effort of achieving the objectives of each decomp, the overall objective of the production of FDCA is achieved.

2.2 Product and Market Research

The purpose of product and market research is to gain an understanding of the production of 2,5-furandicarboxylic acid (FDCA) and its market. It will begin by identifying the chemical structure of 2,5-furandicarboxylic acid (FDCA) and the strengths and weaknesses this structure brings about, as well as the chemical and physical properties that offer an edge when comparing with other products. With the information gathered, a comparison of the properties of 2,5-furandicarboxylic acid (FDCA) to 1,4-dicarboxybenzene which is being commonly used in the current practice. Then, there will also be a researching for proposed synthesis methods used in the production of 2,5-Furandicarboxylic acid (FDCA). In addition, I will also be examining the potential of the derivative of 2,5-furandicarboxylic acid (FDCA), as well as its strengths and weaknesses, since its secondary products are often used in various manufacturing industries and might have tremendous business prospect. Lastly, the research on the current development of 2,5-furandicarboxylic acid (FDCA)

across the globe and the assessment given by major players in the global market to assist in my own analysis is also included.

2.3 Financial Analysis

The financial analysis interprets the production of FDCA with estimated costs, net sales, and net present value. The estimated costs are comprised of production associated costs such as direct labor cost, material cost, indirect overhead, and incidental costs. The net sales are based on the estimated unit price of FDCA of thousand scale and ten thousand scale respectively. Lastly, the net present value calculates the difference between projected earnings generated by the production of FDCA and the anticipated costs, indicating profitability of FDCA within a period of time. Such financial analysis provides statistical interpretation into the production of FDCA.

2.4 Legal Analysis

It is the nature of manufacturing companies to develop distinctive industrial designs catered to the strengths and weaknesses of the company. Often times, companies choose to work with research teams to develop their own manufacturing process, and at the same time, compensate the efforts of the research team. The legal analysis is dedicated to identify ways to legally employ the production method proposed by the research team the company is working with without infringing intellectual property rights.

Chapter 3 -- Results

After conducting a series of research and analysis, it was found out that the potential market for FDCA is massive and it is industrially feasible to manufacture FDCA using fructose as the raw material and several other catalysts and solutions. FDCA as a bio-based building block has an edge in polymerization on fossil-based counterparts in areas such as improved barrier property, higher mechanical strength. Its product in the secondary market also exhibits the above qualities and pose a real threat to the existing market of PET. In addition, FDCA's chemical nature allows it to be "greener" and more environmental-friendly. The financial analysis also suggests that it is profitable to produce FDCA on the thousand ton scale and although more information needs to be acquired to determine the exact profitability of FDCA on the ten thousand ton scale, based on the current analysis, the net present value for FDCA is positive, indicating the production of FDCA is profitable. The legal analysis discussing the possibilities to avoid intellectual property infringement includes two ways: 1) buying out the research findings 2) employing the research team. All these analyses combined were able to validate the future of FDCA and confirm the production of FDCA is a project that is worth investing in.

Chapter 4 -- Discussion

4.1 Axiomatic Design

4.1.1 Overview

The former head of Mechanical Engineering at Massachusetts Institute of Technology and past president at KAIST, Nam Pyo Suh, developed axiomatic design in 1990 (Suh 1990). Dr Suh's rationale for developing axiomatic design was to identify the similarities of all good designs and construct a universal methodology to approach various types of designs. Axiomatic design is a systems design methodology using matrix methods to systematically analyze the translation of customers needs into functional requirements, design parameters, and process variables. It has turned out to be extremely useful for numerous designs, especially in the fields of manufacturing, organizations and software because the two axioms maintain the independence of the functional requirements (FRs) and minimize the information content of the design. It helps simplify complex problems and improve designs.

Axiomatic design employs a systematic design methodology that provides two axioms determining the analysis and decision making process when developing high quality product or system designs. The two axioms used in Axiomatic Design (AD) are:

- Axiom 1: The Independence Axiom; maintain the independence of the functional requirement (FRs).
- Axiom 2: The information axiom; minimize the information content of the design.

The axiomatic design process includes applying these two axioms to provide the best solutions possible for a given set of functional requirements. For this project, the top-level functional requirement was to produce FDCA from biomass.

Any type of manufacturing or system designing problems involve the discussion of maximizing the value added and minimizing the non-value added time so that the overall process could turn out to be as effective and efficient as possible. Providing a solution that maximizes the value added allows the system to reach closer to a robust and potent solution, while minimizing the non-value-added time avoids the involvement of unnecessary and wasteful components that do not play a role in fulfilling the functional requirements. The main goal of lean manufacturing is to minimize waste.

Axiomatic design employs hierarchical design decomposition. Design decompositions exist in domains that report to the goals of the design. These domains address the what and how of the design (Benavides 2012). The domains used in this project are customer domain, functional domain, physical domain, and process domain.

The function domain is characterized by functional requirements (FRs) and constraints. The functional domain translates the customer needs into a much more technical language and represents how the designer interprets the problem given by the customer. Functional requirements satisfy the customer's needs based on the designer's interpretation of the design objectives. The hierarchical nature of axiomatic design instructs the functional requirement to be decomposed into sub-functional

requirements. Each sub-functional requirement must satisfy the original requirement. These sub-functional requirements must be collectively exhaustive that they cover each and every aspect of the manufacturing process, mutually exclusive that there is no overlap between functional requirements, and at a minimum number that the entire process is simplified to the fullest. The best designs maintain the independence of the functional requirements. Consequently, designs have constraints that limit the functional requirements because they might impact a functional requirement's independence. Such constraints, nonetheless, do not have to be independent from each other, and there are two types of constraints involved in axiomatic design: input constraints and system constraints. The input constraints take effect on design conditions while system constraints have an effect on how the design operates.

The physical domain is comprised of design parameters (DPs). The physical domain breaks down the FRs and their constraints into physical properties. Design parameters explain how the design will fulfill functional requirements. Each design parameter is selected to fulfill ideally a single functional requirement for the best compliance with Axiom one, maintaining the independence of functional requirements. These design parameters play a significant role in an item's cost or processes, its physical design, and its development through the design process.

The process domain is comprised of the details of the design parameters. They present a way to produce elements in the physical domain, and in doing so, satisfying the physical properties of a design. The process domain is used for the production of the design.

The independence axiom is used to avoid coupling between FRs and DPs. The presence of coupling in a design can potentially create unpredictability and make the design difficult to adjust and control. Therefore, each functional requirements have its own corresponding design parameter. The design equation stating the relationship between the FRs and DPs may be presented in a matrix.

$$FR = \{X\} * DP$$

Matrix X is known as the design matrix. The design matrix states whether the independence axiom is satisfied. When the design is uncoupled, all of the interactions between the FRs and DPs can be organized to be lower triangular and below the diagonal of the design matrix (Towner, 2013). The diagonal design indicates that each design parameter can satisfy its corresponding functional requirement independently without coupling. If the design matrix is lower triangular, the design is then considered to be decoupled, indicating that it can satisfy the independence axiom if the order of adjustment is correctly chosen (Catherine Asenso, Jacqueline Foti, David Liston & Kristin Smith, 2013). However, when a design matrix is not diagonal or triangular, it is considered to be coupled, indicating that there is no arrangement of FD and DP matrix can satisfy the functional requirements independently.

Uncoupled Design

$$\begin{bmatrix} FR1 \\ FR2 \\ FR3 \end{bmatrix} = \begin{bmatrix} X11 & 0 & 0 \\ 0 & X22 & 0 \\ 0 & 0 & X33 \end{bmatrix} * \begin{bmatrix} DP1 \\ DP2 \\ DP3 \end{bmatrix} \rightarrow \begin{matrix} FR1 = X11 * DP1 \\ FR2 = X22 * DP2 \\ FR3 = X33 * DP3 \end{matrix}$$

Figure 1: Uncoupled Design

Decoupled Design

$$\begin{bmatrix} FR1 \\ FR2 \\ FR3 \end{bmatrix} = \begin{bmatrix} X11 & 0 & 0 \\ X21 & X22 & 0 \\ X31 & X32 & X23 \end{bmatrix} * \begin{bmatrix} DP1 \\ DP2 \\ DP3 \end{bmatrix} \rightarrow \begin{aligned} FR1 &= X11 * DP1 \\ FR2 &= X21 * DP1 + X22 * DP2 \\ FR3 &= X31 * DP1 + X32 * DP2 + X33 * DP3 \end{aligned}$$

Figure 2: Decoupled Design

Coupled Design

$$\begin{bmatrix} FR1 \\ FR2 \\ FR3 \end{bmatrix} = \begin{bmatrix} X11 & X12 & X13 \\ X21 & X22 & X23 \\ X31 & X32 & X23 \end{bmatrix} * \begin{bmatrix} DP1 \\ DP2 \\ DP3 \end{bmatrix} \rightarrow \begin{aligned} FR1 &= X11 * DP1 + X12 * DP2 + X13 * DP3 \\ FR2 &= X21 * DP1 + X22 * DP2 + X23 * DP3 \\ FR3 &= X31 * DP1 + X32 * DP2 + X33 * DP3 \end{aligned}$$

Figure 3: Coupled Design

(Catherine Asenso, Jacqueline Foti, David Liston & Kristin Smith, 2013)

4.1.1.1 Design Software

The design software used for this project is Acclaro®DFSS. It is a software developed by Axiomatic Design Solutions, Inc and used often for managing design hierarchy. Acclaro® allows us to show and understand the interaction between functional requirements and design parameters. Each functional requirement has its own sub-functional requirements and combining all of the sub-functional requirements, the overall functional requirement would be achieved. Acclaro® also has a column of design matrix that displays its interactions with respective functional requirement (Axiomatic Design Solutions INC. 2013).

4.1.2 Statement of the highest level functional requirement - FR₀

The goal of this production system is to produce 2,5-Furandicarboxylic acid (FDCA) from biomass. From here, the lower level functional requirements work in sequence to achieve this goal and produce 2,5-Furandicarboxylic acid (FDCA) as the

final product.

4.1.3 Statement of the first level functional requirement - FR₁

The first step of this production system is to extract starch from biomass such as corn stalks because the largest selling point of 2,5-Furandicarboxylic acid (FDCA) is that it is 100% biomass-based and derived entirely from biomass. This practice to extract starch and cellulose from biomass is currently involved with the production of numerous bio-based polyesters and does not present a severe technical obstacle. The main method to achieve this goal industrially is to compile harvest corn stalks and organize them in spherical patterns forming starch granules. Then, when heated in solution, the starch granules absorb water and eventually gelatinize into a paste (Learning Target 2018).

4.1.4 Statement of the second level functional requirement - FR₂

The next step is to extract glucose from the starch. Similarly, this step has been around in the industry for a long time and can be achieved through the use of acid or enzymes. To produce glucose, the starch is treated with acid or enzymes and heated in a conversion process to break down starch molecule, ultimately resulting in the production of a wide variety of glucose (Alif)

4.1.5 Statement of the third level functional requirement -FR₃

The next step is to convert glucose to fructose. This step is achieved by

enzymatic isomerization. Studies have found that some strains of *Streptomyces* species have been found to produce isomerase that has catalyzed a conversion of glucose to fructose. Such enzyme from *Streptomyces* with high yield, heat-tolerance and strong activity presented advantages to other microbial isomerases that promised the possibility of industrial production of isomerized sugar such as fructose. There is another study that found the possibility to chemically isomerize fructose that includes high temperature reaction condition and the stop of reaction in a very short time to avoid sugar destruction. This process guarantees industrially acceptable yield of fructose (around 35%) and unimaginably low sugar destruction to color substances and organic acids (Shigeo Suzuki, Nobuzo Tsumura, 1972). Both methods are being used in the industry to convert glucose to fructose and proven effective in the field.

4.1.6 Statement of the fourth level functional requirement -FR₄

The next step is to acquire HMF from fructose. This is the step that is still under experiment because HMF is usually not stable under current practice after production to be oxidated into the final product FDCA or the production process involves the use of raw materials that are too expensive to justify the production process. The industry has not yet to identify a universally feasible approach to industrially and economically produce stable HMF that is ready for the next stage of oxidation. However, the manufacturing of HMF fundamentally determines if it is possible to mass produce FDCA as it is the precursor of FDCA and researchers are focusing on finding the adequate catalyst and reaction environment to make it happen. This will be explained

more in depth in Chap. 4.

4.1.7 Statement of the fifth functional requirement -FR₅

The last step is to oxidate HMF and produce FDCA. This is another step that has not been entirely agreed upon yet. There are now two different approaches to perform this procedure: aqueous-phase oxidation and organic-phase oxidation. The aqueous-phase oxidation is a fairly mature production method and its safety has been proven, while the organic-phase oxidation is still under development but has the potential to drastically reduce the cost of production. The safety of organic-phase oxidation is another issue that garners our attention. The method that utilizes aqueous-phase oxidation has ensured that it is possible to oxidate HMF and organic-phase oxidation presents a new opportunity to reduce the cost. Both methods will be compared more in details in Chap.5

4.1.8 Completed Axiomatic Design Hierarchy

The completed decomposition is shown in the figure below. It includes all of the functional requirements and design parameters.

#	[FR] Functional Requirements	[DP] Design Parameters
0	Produce FDCA from corn stalks/biomass	Industrial design that produces FDCA from corn stalks/biomass
1	Acquire starch/cellulose from corn stalks	System to acquire starch by gelatinizing heated starch granules
2	Extract glucose from the starch/cellulose	System to acquire Glucose from Starch/Cellulose through Hydrolysis
3	Convert glucose to fructose	System to acquire Fructose from Glucose through Isomerization
4	Acquire HMF from fructose	System to acquire HMF from Fructose through Dehydration
5	Produce FDCA from HMF	System to acquire FDCA from Oxidation

Figure 4: Design Hierarchy

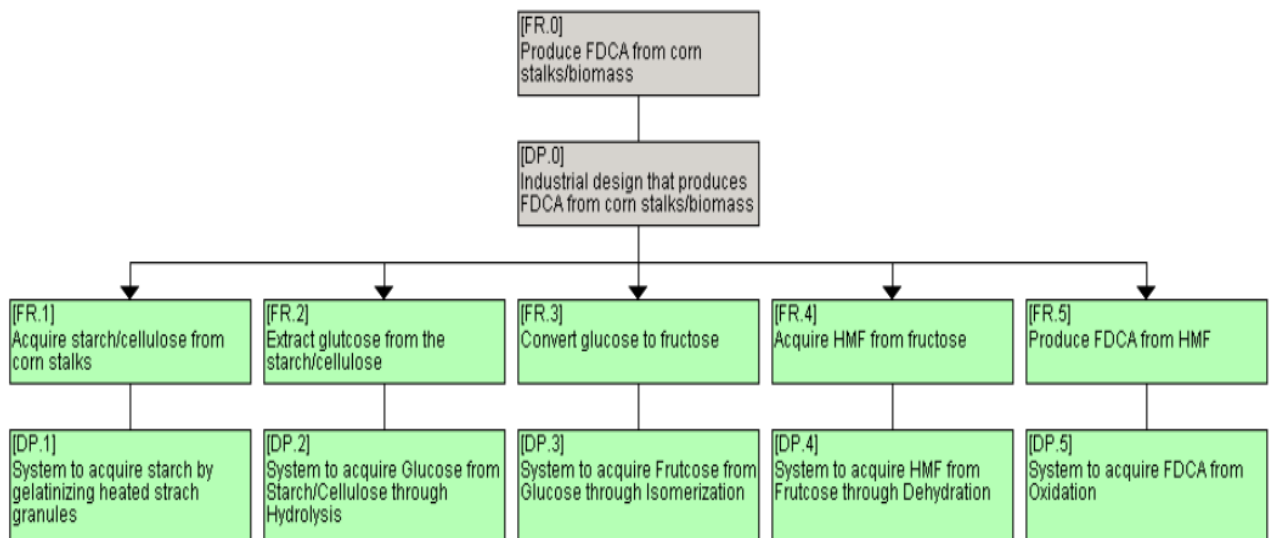


Figure 5: Design Hierarchy Tree

4.1.9 Interactions between the top level DPs and FRs

To fulfill FR1, the design needs to extract starch from biomass such as corn stalks; this FR is satisfied through DP1 which is a system that heats up the corn stalks placed in solution. To fulfill FR2, the design needs to extract glucose from starch; this FR is satisfied through DP2 which is a system that uses acid or enzymes to produce in heated solution. To fulfill FR3, the design needs to convert glucose to fructose; this

FR is satisfied through DP3 which is a system that chemically or enzymatically produce isomerized sugars such as fructose. To fulfill FR4, the design needs to acquire HMF from fructose; this FR is satisfied through DP4 which is a system that achieves that objective through dehydration with various catalysts. To fulfill FR5, the design needs to acquire the final product FDCA from HMF; this is satisfied by oxidating HMF through either aqueous-phase oxidation or organic-phase oxidation.

Since all of the FRs listed above have to take place in sequence, FR₁ needs to be satisfied prior to FR₂, and FR₂ needs to be satisfied prior to FR₃ and so on because if the product of the previous functional requirement was not manufactured first, the material to produce the product of the present functional requirement would not exist in the first place, rendering the entire procedure impossible. This association is known as uncoupled design.

4.1.10 Completed Design Matrix

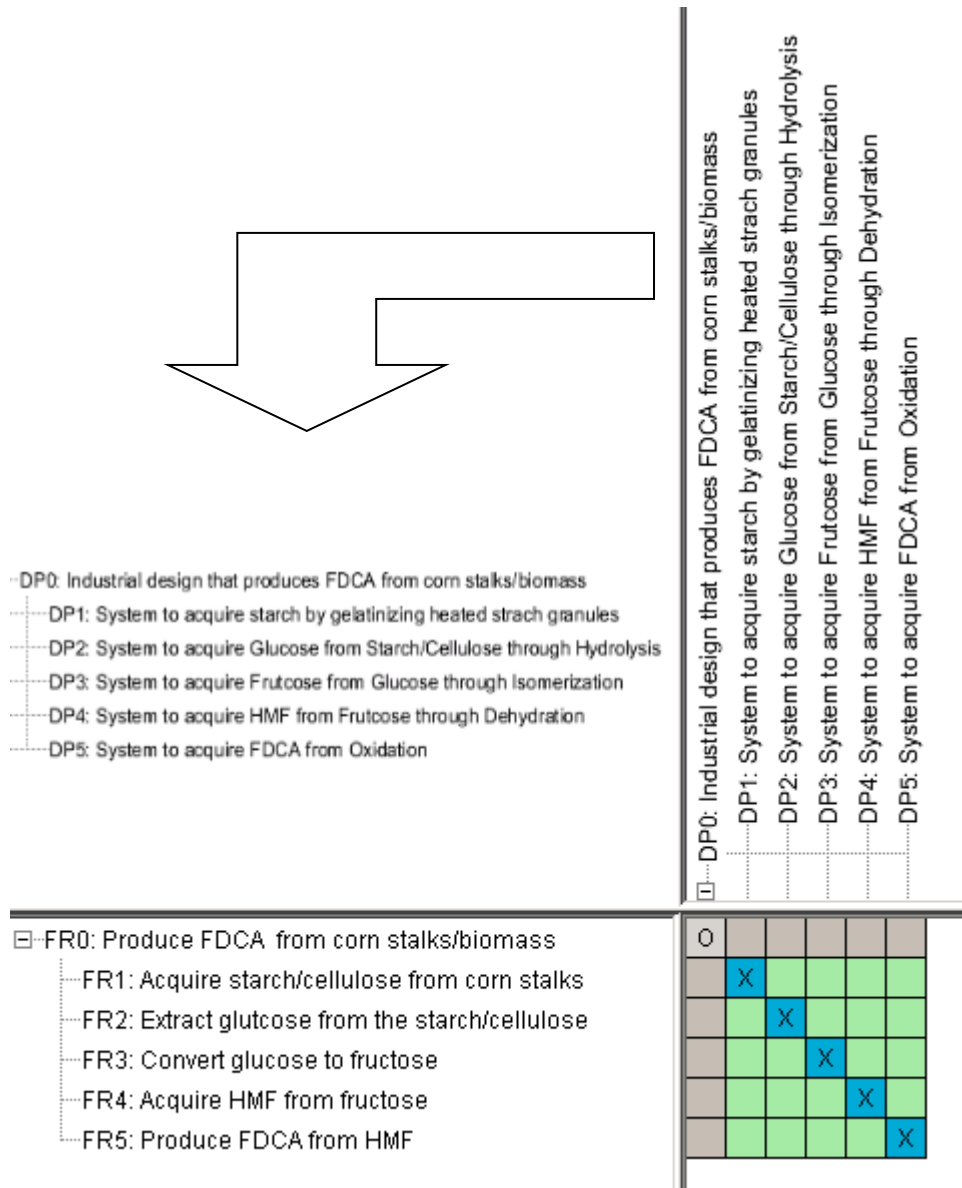


Figure 6: Design Matrix

4.2 Product and Market Research

4.2.1 FDCA Product Description

2,5-Furandicarboxylic acid (FDCA) is an organic compound consisting of two carboxylic acid groups attached to a central furan ring. It is considered to be a renewable resource because it can be produced from certain carbohydrates. 2,5-Furandicarboxylic acid (FDCA) was identified by the U.S. Department of Energy as one of 12 priority chemicals for establishing the “green” chemistry industry of the future (Royal Society of Chemistry, 2010). 2,5-Furandicarboxylic acid (FDCA) has been suggested as an important renewable building block because it can substitute for terephthalic acid (PTA) in the production of polyesters and other current polymers containing an aromatic moiety. With the appropriate production methods, 2,5-Furandicarboxylic acid (FDCA) has tremendous potential in the production of every day products, including water bottle that influence our daily lives from all aspects.

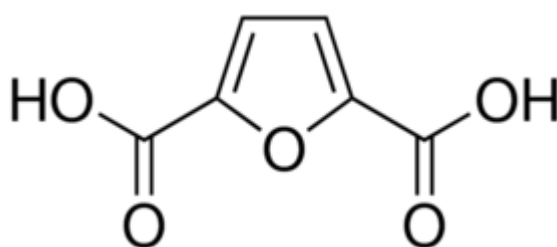


Figure 7: FDCA Chemical Structure

2,5-Furandicarboxylic acid (FDCA) is a very stable compound, and its physical properties, such as insolubility in most of common solvents and a very high melting point (342°C) seem to indicate intermolecular hydrogen bonding. Despite its chemical

stability, 2,5-Furandicarboxylic acid (FDCA) undergoes reactions typical for carboxylic acids, such as halogen substitution to give carboxylic dihalides, the di-ester formation and the formation of amides (Lewkowski J. 2001).

4.2.1.1 SWOT Analysis

The main goal and objective for FDCA is essentially to challenge or replace the role of PTA in the production of PET. FDCA can be used as a building block to produce PEF that has the potential to challenge the market of PET. The market of PET has been around for decades and presents obstacles for the introduction of FDCA. Therefore, in order to gain a better understanding of FDCA, a SWOT analysis was prepared to determine the chemical strengths and possible benefits for the product. This would not only facilitate in justifying the research and development of FDCA, but also would it aid in the decision of moving forward with the production of FDCA and an appropriate marketing plan.

Strengths

The strengths of FDCA are numerous. First of all, the most important property of FDCA is that it is bio-based and can be directly manufactured from corn stalks. This provides a chemical edge and adheres to the international mission of “going green”. The potential market for a sustainable alternative to fossil-based polyesters is huge and very promising. In addition, FDCA also has superior performance criteria, such as improved barrier properties and higher mechanical strength that allows it to become

the main building block for producing bio-based products through polymerization.

Weaknesses

Even though the market potential is huge and the results of FDCA are almost guaranteed once the research is completed, no one can be sure if FDCA can truly live up to its expectation. In the current stage, there has only been reports showing that it is possible to produce FDCA in the lab and can potentially be scaled up to an industrial level and produce profits. However, the production stability and whether FDCA can really achieve its expectation are still yet to be resolved because in the pharmaceutical industry, scaling up a substance or drug can be much more complicated than mathematical multiplication. There are various types of issues that might occur when producing products industrially and it is only when the production method has been proven to be successful, can the product be considered profitable. Also, since the production of FDCA is still at an experimental stage, the details of production are still premature and vary greatly from companies to companies. This uncertainty in its manufacturing methods creates risks, consequently affecting the cost-to-benefit analysis in a way that it is still an estimation and regardless of how precise these estimations come close to the reality, we still need to leave some room for doubt until proven otherwise. There are always risks involved that need to be taken into account for novice products such as FDCA itself.

Opportunities

The outstanding barrier properties and other chemical strengths have created a

tremendous amount of opportunities for FDCA and its secondary market. For starters, the most important product in the secondary market is PEF. PEF is a 100% recyclable, bio-based polymer. PEF has great potential in replacing the currently extensively utilized polymer PET because PET is fossil-fuel-based and lacks renewability. The production method of PEF is straightforward and mimics the production of PET with the only difference of FDCA replacing PTA. The flow chart below compares the synthesis of PET and PEF.

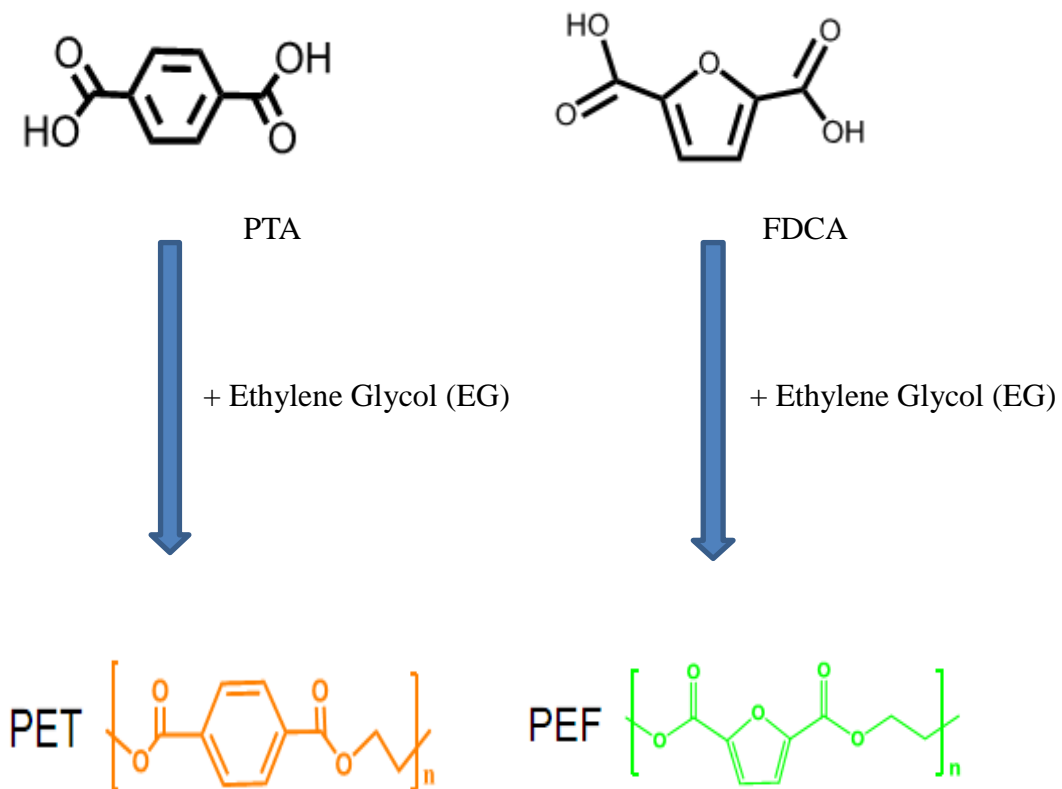


Figure 8: PET v.s. PEF

Some of the superior barrier properties of FDCA include: 1) PEF's oxygen barrier is 10 times better than PET 2) PEF's carbon dioxide barrier is 6 to 10 times better than PET 3) PEF's water barrier is twice as good as PET's. PEF also has more attractive

thermal properties such as the glass transition temperature (the temperature when plastics start turning to a viscous or rubbery state from a glassy state) is 86°C compared to the glass transition temperature of PET of 74°C and the melting point of PEF is 235 °C compared to that of PET of 265 °C, which also creates an extensive amount of opportunities in industrial plastics, including bottles, textiles, food packaging, carpets, electronic materials and automotive applications (Aantium, 2018). The introduction of FDCA , along with PEF, is expected to challenge the market PET as a greener alternative of industrial polymer with better performance.

In addition, with countries all over the world actively advocating the reduction of emitting carbon dioxide and leading humanity on a “greener” path, the advent of FDCA and its secondary products will provide more opportunities that dovetail the global mission of “going green”.

Threats

Although FDCA is such a promising product that obviously has gathered a lot of attention in the industry, the fact that it is still relatively new and its production methods are premature presents some real threats to consider for the future of FDCA.

As much as PET is less environmental-friendly, it is a market that has been around for decades and proven to be successful. For a new product such as FDCA itself to invade and challenge an existing market, the risks and difficulties should never be understated. The major issue with PEF challenging PET is that every aspect of PET from sourcing to production and sales are all determined and finalized to

details, while some aspects of PEF are still up in the air and no one can be sure of the outcome of investing in PEF or FDCA. The risks for a company to carry on producing PET is relatively small compared to that of PEF. However, in the world of business, with greater risks come greater benefits, and this is just something companies should contemplate and decide on their own.

Furthermore, as in the aforementioned sections, the fact that the production methods of FDCA varies from companies to companies creates threats. In the current stage, companies are all endeavoring to identify the cheapest and most effective way to produce FDCA. Nonetheless, when someone else in the industry figures out a better approach to manufacture FDCA, it presents threats for all other participants in the market. It is the nature of manufacturing industry that everyone is looking to produce more high-quality products within a shorter period of time and with less investment. This threat of not having a technical edge will always be present as long as the company is in the manufacturing industry and can not be truly resolved once and for all.

<p>Strengths</p> <ul style="list-style-type: none"> ▪ Can be used as building block ▪ Good barrier properties and high mechanical strength ▪ Renewable and green 	<p>Weaknesses</p> <ul style="list-style-type: none"> ▪ Production method, costs and production stability on n industrial level are not determined ▪ Not sure if the high expectation can be achieved
<p>Opportunities</p> <ul style="list-style-type: none"> ▪ PEF ▪ Other secondary products such as food packaging, bottles, and textiles. ▪ Adheres to the mission of “going green” 	<p>Threats</p> <ul style="list-style-type: none"> ▪ Going to challenging the market of PET ▪ Other market participant’s improvement on production method.

Table 2: SWOT Analysis

4.2.2 Synthesis of FDCA

4.2.2.1 Overview

The methods for the synthesis of the FDCA is widely believed to be divided into four groups in the industry (Lewkowski J. 2001):

- 1) Dehydration of hexose derivatives
- 2) Oxidation of 2,5-disubstituted furans
- 3) Catalytic conversions of various furan derivatives

4) Biological conversion of HMF

Dehydration of hexose derivatives

First group is based on the acid-promoted triple dehydration of aldaric acid. This reaction asks for rigorous conditions (highly concentrated acids, temperature higher than 120 °C, reaction time longer than 20 hours) and all the methods were non-selective with yields that are lower than 50% (Y. Yaguchi, A. Oishi and H. Lida, 2008). The process has also been patented by the French company Agro Industrie Recherches et Developpements, and this is also the process which DuPont and ADM are using according to patent literature (Biofuels Digest, 2016).

Oxidation of 2,5-disubstituted furans

The second group of synthesis routes incorporate the oxidation reactions of various 2,5-disubstituted furans utilizing a variety of inorganic oxidants. The industry has recognized several routes to FDCA via oxidation of hydroxymethylfurfural (HMF) with air over different catalysts. Oxidation of HMF under strongly alkaline conditions over noble metal catalysts gives almost quantitative formation of FDCA (P. Verdeguer; N. Merat; A. Gaset, 1993). HMF and methoxymethylfurfural (MMF) oxidation was also studied with a series of conventional metal bromide catalysts (Co, Mn, Br) used for the oxidation of para-xylene to terephthalic acid.

Catalytic conversions of various furan derivatives

The third group includes reactions explaining the synthesis of FDCA from fufural. Furfural can be oxidized to 2-furoic acid with nitric acid and the latter was subsequently converted to its methyl ester. Then, the ester was then converted via chloromethylation at position 5 in order to produce 5-chloromethylfuroate, which was then oxidized with nitric acid to form dimethyl 2,5-furandicarboxylate. Lastly, after the alkaline hydrolysis, FDCA resulted in a 50% yield (Andrisano, 1963). It was also reported that potassium 2-furoate, when heated up to 300 degrees celcius in a nitrogen atmosphere, would undergo decarboxylation to furan with simultaneous carboxylation at position 5 to dipotassium 2,5-furandicarboxylate.

Biological conversion of HMF

FDCA has also been discovered in human urine. A healthy human produces 3-5mg/day of FDCA. Numerous reports have been performed to establish the metabolism of this compound and to determine its quantity, which is usually produced depending on the healthiness of the human. Reports have also found that the individual quantity of produced FDCA increased after the intake of fructose. FDCA was also detected in blood plasma (Lewkowski J. 2001). Recently, the enzyme furfural/HMF oxidoreductase was isolated from the bacterium *Cupriavidus basilensis* HMF 14, which is able to convert HMF to FDCA using molecular oxygen. A *Pseudomonas putida* strain that was genetically engineered to express this enzyme has the ability to completely and selectively convert HMF to FDCA. This biocatalysis is performed under very environmental friendly conditions. Water at ambient

temperature and pressure will be able to commence the conversion without producing toxic or polluting chemicals.

Technical Barriers

Aforementioned are the four main groups that are discussed and considered to be the methods to produce FDCA. However, the industrially viable solution is still being researched and experimented because the primary technical barrier in the production and use of FDCA is the development of an effective and selective dehydration process from sugars. The technology to control sugar dehydration could potentially be very powerful and leading to a wide range of additional, cost effective building blocks. The fact that it is still yet to be well understood causes difficulties in the production of FDCA. Under currently practice, dehydration processes using hydroxymethylfurfural (HMF) as intermediate are generally non-selective, unless the unstable intermediate products can be immediately transformed into more stable materials such as methoxymethylfurfural (MMF) immediately upon its formation. R&D is still developing selective dehydration systems and catalysts to come up with a inexpensive and industrially viable oxidation technology that can operate jointly with the necessary dehydration processes.

4.2.2.2 Recent Reports

While the previous section explains four main possible approaches that we might be able to produce FDCA from a chemical and structural standpoint, some of the

methods have turned out to be less cost efficient (involving the use of expensive raw material) or too chemically unstable to carry out. It is still possible that major breakthrough occurs and solve these types of problems. However, more practical experiment and research have been focusing on searching for efficient catalysts, processing conditions to prepare FDCA in an environmentally benign solvent and the catalytic oxidation process of HMF as they follow the generally agreed synthesis route, which includes the dehydration of fructose and the oxidation of HMF to yield FDCA.

In this section, I'll be describing several feasible way to industrially produce FDCA with acceptable yields.

Pd/CC catalyst



Figure 9: Pd/CC Catalyst

Pd/CC catalyst was synthesized from readily available biomass-derived D-glucose. It has shown excellent catalytic activity toward the synthesis of FDCA from HMF and fructose. Oxidation of HMF resulted in 85% yield, and dehydration of fructose

followed by oxidation gave 64% yield of FDCA with 100% purity using Pd/CC catalyst and molecular O₂ as an oxidizing agent under aqueous reaction conditions. This one pot two step procedure is extremely efficient for the synthesis of FDCA from fructose because it neglects the isolation of HMF, which is chemically unstable, and requires only a single catalyst for two distinctive steps.

Fe-Zr-O catalyst

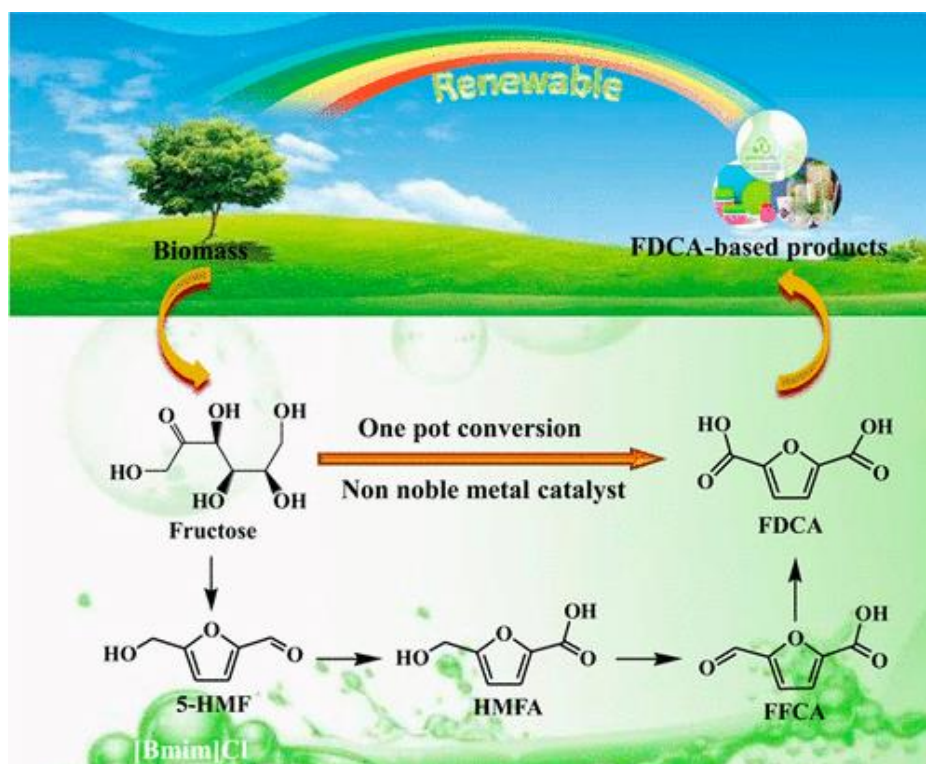


Figure 10: Fe-Zr-O Catalyst

Instead of using noble metal catalysts, this approach employs Cl as solvent with non-noble metal (Fe-Zr-O) as a catalyst in order to reduce the high costs of starting material and catalysts. Under optimal conditions, relatively high FDCA yield was obtained at full fructose conversion. This study has also shown that the oxidation of

intermediate FFCA to FDCA required the highest activation energy, indicating this step is highly subject to reaction temperature. In addition, in this reaction system, other biomass sources, such as glucose, galactose, mannose, starch, and cellulose can also be directly converted only with lower FDCA yield in comparison to that of fructose because of the ineffective isomerization of aldohexoses into fructose.

GVL/H₂O solvent system and Pt/C catalyst

This method reported a process of converting fructose at a high concentration (15 weight %) to FDCA. In this process, fructose is dehydrated to HMF at a yield of 70% using a γ -valerolactone (GVL)/H₂O solvent system. HMF is then oxidized to FDCA over a Pt/C catalyst, which is essentially another form of the use of noble metal, with 93% yield. The strength of this system is the higher solubility of FDCA in GVL/H₂O, allowing oxidation at high concentrations using a heterogeneous catalyst that eliminates the need for a homogeneous base. The other aspect that makes this method possible is that FDCA can be separated from the GVL/H₂O solvent system by simple crystallization to obtain >99% pure FDCA.

Aerobic oxidation over supported metal catalysts

This method involves the use of supported metal catalysts, in this case Pt catalysts. Under the optimum reaction conditions of a stepwise increase in the reaction temperature (75 and 140 degrees celsius for 12 hours each). the report claimed that they achieved as high as 96% FDCA yield in presence of 1 bar oxygen pressure over

Pt/ γ -Al₂O₃. Researchers have also found that that as oxygen pressure increases (1-10 bar), the yield of FDCA tended to decrease because overoxidation reactions of substrate and products are possible at higher partial pressure of oxygen. What is especially important for this method is that even with air as an oxidant, researchers have obtained similar yields of FDCA as that with oxygen, indicating such method could be implemented without having to use oxygen and consequently simplify production process and reduce cost. Furthermore, confirmed by NMR, melting point, and elemental analysis, FDCA formed in this reaction can be successfully isolated (91%, isolated yield) in the pure form.

4.2.3 Competition Evaluation

As of right now, there is not much information to be found on the development of FDCA since it is still in an experimental stage and the information is all classified. However, according to the publication from some of the major market participants and forerunners in the industry, they have been gradually making progress towards the goal of industrially producing FDCA and potentially generate competition in the long run. Below is a chart that summarizes the progress of some of the leading companies in the manufacturing of FDCA.

Company/Or ganization	CNITEC H	USTC	DuPont	ADM	Avantium	AVABIOC HEM
Country	China	China	U.S.	U.S.	Netherlands	Switzerland
Collaborator	None	None	ADM	DuPont	BASF/Coca Cola	None
Current Development	100t/yr	100t/yr	60t/yr (under construction)		40t/yr	20t/yr
Method	water phase/ water phase	water phase/ water phase	tert-Butyl alcohol/acetic acid		methanol/ acetic acid	water phase/acetic acid
Construction Goal	1000t/yr	Unknown	Unknown		50000t/yr	120000t/yr

Table 3: Competition Evaluation

4.3 Financial Analysis

In order to quantify the Net Present Value, the ‘NPV’ of two different production scales on a five-year plan was calculated to help in making the decision of whether the company should move forward with the production of FDCA. Since the production of fructose is fairly mature and well-developed, the company has decided, instead of manufacturing directly from biomass, to purchase and use fructose as the

raw material to manufacture FDCA to simplify the manufacturing process and reduce costs.

Below are two cash flow diagrams for the thousand ton scale and the ten thousand ton scale respectively.

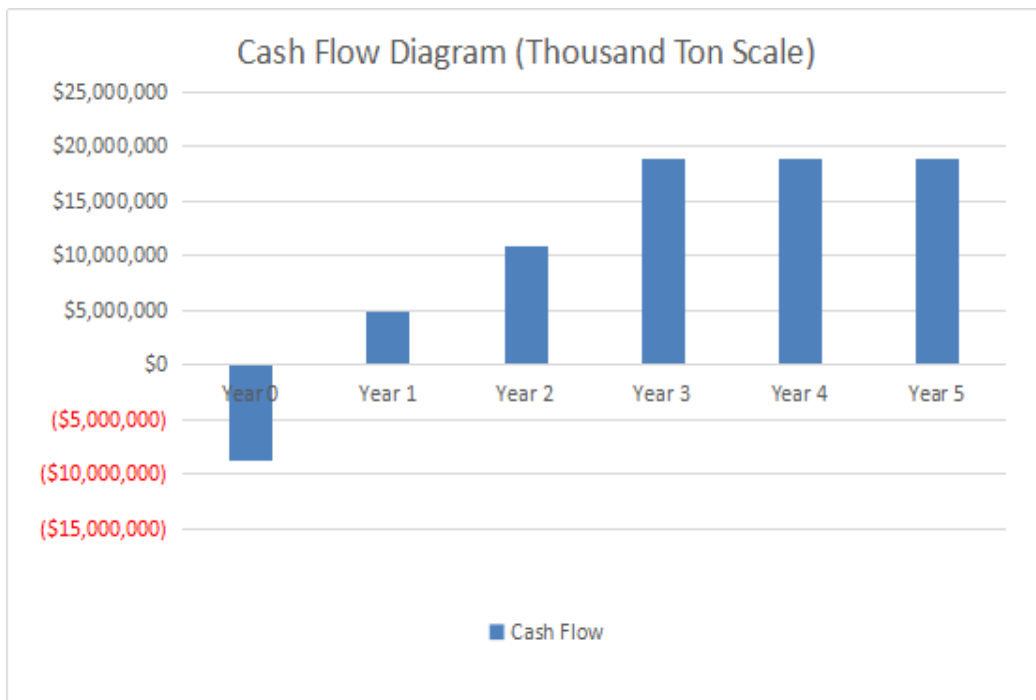


Figure 11: Cash Flow Diagram (Thousand Ton Scale)

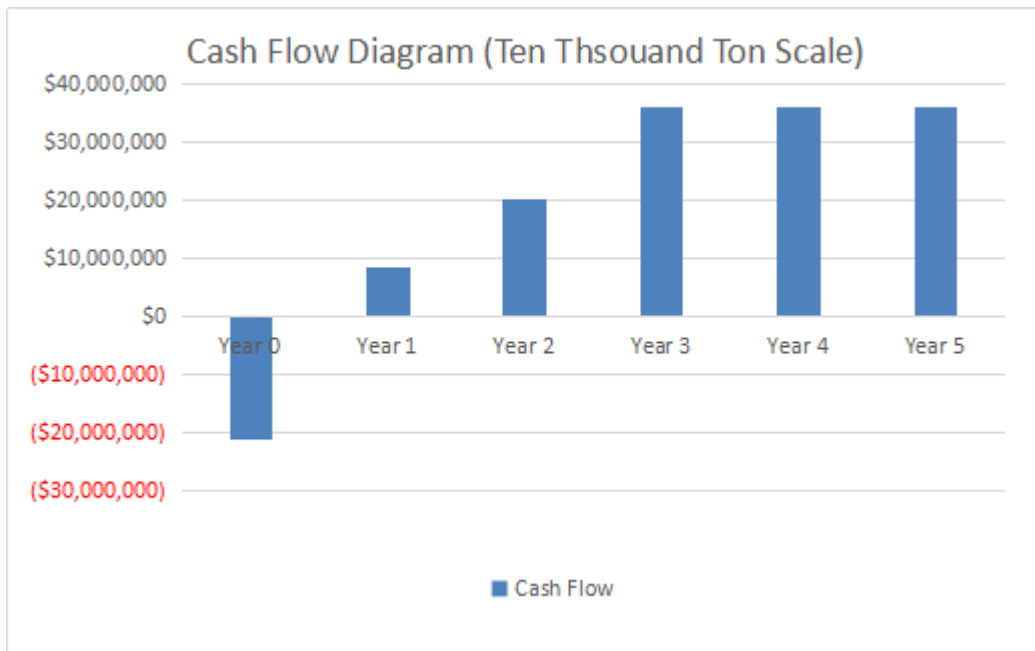


Figure 12: Cash Flow Diagram (Ten Thousand Ton Scale)

4.3.1 Expenses

Based on the sequence of procedures and potential costs that are expected to occur during the manufacturing process, a cost analysis of different scales of production was conducted and presented as follows. The thousand ton scale is also considered to be the “midsize trial” because it is the first time the company tries to scale up the production of FDCA from an experimental stage to an industrial level. However, it is not upon the completion of the “midsize trial”, can the company make a more precise estimation towards the ten thousand ton scale because the data and feedback acquired from the “midsize trial” will also contribute to the cost analysis of the ten thousand ton scale production of FDCA. The current estimated costs for the ten thousand ton scale is mainly for the purpose of comparing with the “midsize trial” and are subject to change once more information is acquired. The detailed estimated

costs for Thousand Ton Scale and Ten Thousand Ton Scale are shown below.

		Thousand Ton Scale						
	Production Quantity (Ton)	Per ton	Year 0 0	Year 1 300	Year 2 600	Year 3 1000	Year 4 1000	Year 5 1000
Expenses			\$8,700,000.00	\$2,651,500	\$4,153,000	\$6,155,000	\$6,155,000	\$6,155,000
Fixed Cost			\$8,700,000.00	\$0	\$0	\$0	\$0	\$0
	R&D		\$1,200,000	\$0	\$0	\$0	\$0	\$0
	Plant Construction		\$7,500,000	\$0	\$0	\$0	\$0	\$0
Direct Labor Cost	30 workers		\$0	\$400,000	\$400,000	\$400,000	\$400,000	\$400,000
Material Cost				\$1,146,000	\$2,292,000	\$3,820,000	\$3,820,000	\$3,820,000
	Fructose	\$1,800	\$0	\$540,000	\$1,080,000	\$1,800,000	\$1,800,000	\$1,800,000
	Catalyst 1	\$10	\$0	\$3,000	\$6,000	\$10,000	\$10,000	\$10,000
	Solution 1	\$900	\$0	\$270,000	\$540,000	\$900,000	\$900,000	\$900,000
	Solution 2	\$1,100	\$0	\$330,000	\$660,000	\$1,100,000	\$1,100,000	\$1,100,000
	Catalyst 2	\$10	\$0	\$3,000	\$6,000	\$10,000	\$10,000	\$10,000
Indirect Overhead				\$115,500	\$231,000	\$385,000	\$385,000	\$385,000
	Cooling Water	\$40	\$0	\$12,000	\$24,000	\$40,000	\$40,000	\$40,000
	Electricity	\$90	\$0	\$27,000	\$54,000	\$90,000	\$90,000	\$90,000
	Steam	\$250	\$0	\$75,000	\$150,000	\$250,000	\$250,000	\$250,000
	Natural Gas	\$5	\$0	\$1,500	\$3,000	\$5,000	\$5,000	\$5,000
Incidental Costs				\$990,000	\$1,230,000	\$1,550,000	\$1,550,000	\$1,550,000
	Depreciation on Equipment		\$0	\$750,000	\$750,000	\$750,000	\$750,000	\$750,000
	Other Cost	\$800	\$0	\$240,000	\$480,000	\$800,000	\$800,000	\$800,000

Figure 13: Expenses (Thousand Ton Scale)

		Ten Thousand Ton Scale						
	Production Quantity (Ton)	Per ton	Year 0 0	Year 1 3000	Year 2 6000	Year 3 10000	Year 4 10000	Year 5 10000
Expenses			\$21,200,000.00	\$14,035,000	\$24,670,000	\$38,850,000	\$38,850,000	\$38,850,000
Fixed Cost			\$21,200,000.00	\$0	\$0	\$0	\$0	\$0
	R&D		\$1,200,000	\$0	\$0	\$0	\$0	\$0
	Plant Construction		\$20,000,000	\$0	\$0	\$0	\$0	\$0
Direct Labor Cost	30 workers		\$0	\$400,000	\$400,000	\$400,000	\$400,000	\$400,000
Material Cost				\$9,510,000	\$19,020,000	\$31,700,000	\$31,700,000	\$31,700,000
	Fructose	\$1,700	\$0	\$5,100,000	\$10,200,000	\$17,000,000	\$17,000,000	\$17,000,000
	Catalyst 1	\$10	\$0	\$30,000	\$60,000	\$100,000	\$100,000	\$100,000
	Solution 1	\$650	\$0	\$1,950,000	\$3,900,000	\$6,500,000	\$6,500,000	\$6,500,000
	Solution 2	\$800	\$0	\$2,400,000	\$4,800,000	\$8,000,000	\$8,000,000	\$8,000,000
	Catalyst 2	\$10	\$0	\$30,000	\$60,000	\$100,000	\$100,000	\$100,000
Indirect Overhead				\$885,000	\$1,770,000	\$2,950,000	\$2,950,000	\$2,950,000
	Cooling Water	\$30	\$0	\$90,000	\$180,000	\$300,000	\$300,000	\$300,000
	Electricity	\$60	\$0	\$180,000	\$360,000	\$600,000	\$600,000	\$600,000
	Steam	\$200	\$0	\$600,000	\$1,200,000	\$2,000,000	\$2,000,000	\$2,000,000
	Natural Gas	\$5	\$0	\$15,000	\$30,000	\$50,000	\$50,000	\$50,000
Incidental Costs				\$3,240,000	\$3,480,000	\$3,800,000	\$3,800,000	\$3,800,000
	Depreciation on Equipment		\$0	\$3,000,000	\$3,000,000	\$3,000,000	\$3,000,000	\$3,000,000
	Other Cost	\$80	\$0	\$240,000	\$480,000	\$800,000	\$800,000	\$800,000

Figure 14: Expenses (Ten Thousand Ton Scale)

Several costs that may occur during the manufacturing process include fixed cost, direct labor cost, material cost, indirect overhead, and incidental expenses.

Fixed Cost			\$8,700,000.00
	R&D		\$1,200,000
	Plant Construction		\$7,500,000

Figure 15: Fixed Cost (Thousand Ton Scale)

Fixed Cost			\$21,200,000.00
	R&D		\$1,200,000
	Plant Construction		\$20,000,000

Figure 16: Fixed Cost (Ten Thousand Ton Scale)

Due to the fact that the research of FDCA’s production method is still underway and the company is working closely with a research team to determine the final production route, they are expected to continue investing into this project from 6 months to 1 year for an estimated total of \$1,200,000. This investment of research and development is a sunk cost that cannot be recovered once incurred. It is also interpreted as a fixed cost because regardless of the units of product the company is looking to produce, this cost of research and development remains the same and is the first step before moving forward. In addition, this cost is independent from the scale of production because it is not directly part of the production process. The plant construction costs for the thousand ton scale and the ten thousand ton scale are different with the first one being \$7,500,000 and the latter being \$20,000,000. The ten thousand ton scale is capable of producing FDCA on a larger quantity, which also

demands for a larger investment in the beginning. This cost of research and development, as well as the plant construction cost, will occur during the Year 0, which is a year before actual production will commence.

The direct labor cost is the same for both the thousand ton scale and the ten thousand ton scale. For the thousand ton scale, also known as the “midsize trial”, even though the addition of material and the reaction pot are both automated . Three teams of 10 workers each working in shifts are required to participate in activities such as overseeing the operation of machinery, warehouse cleaning, and maintenance, which accounts for the salaries and appropriate benefits for a total of 30 workers. Although in this five-year plan, the company is going to gradually build up their production quantity to full capacity for both scales, the number of workers working in the plant will remain the same throughout five years, and this boils down to \$400,000 a year to complete the production of FDCA on a thousand ton scale. When scaling the manufacturing up to ten thousand level, the production route remains basically the same, and the only difference is that the machinery is designed to complete the same reaction on a larger quantity. The reaction pot is continuous and 100% automated as well. Although the reaction machinery might be larger in size, the size of the team does not have to grow at all. The same amount of three teams of 10 workers each working in shifts are sufficient to complete the same tasks.

The material costs include fructose, catalyst 1, catalyst 2, solution 1, and solution 2. Because of the marginal effect, the unit costs of each material vary depending on the scale of production. As for thousand ton scale, the material costs are listed as

follow.

	Per ton	Year 0	Year 1 (300t)	Year 2(600t)	Year 3(1000t)	Year 4(1000t)	Year 5(1000t)
Material Cost			\$1,146,000	\$2,292,000	\$3,820,000	\$3,820,000	\$3,820,000
Fructose	\$1,800	\$0	\$540,000	\$1,080,000	\$1,800,000	\$1,800,000	\$1,800,000
Catalyst 1	\$10	\$0	\$3,000	\$6,000	\$10,000	\$10,000	\$10,000
Solution 1	\$900	\$0	\$270,000	\$540,000	\$900,000	\$900,000	\$900,000
Solution 2	\$1,100	\$0	\$330,000	\$660,000	\$1,100,000	\$1,100,000	\$1,100,000
Catalyst 2	\$10	\$0	\$3,000	\$6,000	\$10,000	\$10,000	\$10,000

Figure 17: Material Costs (Thousand Ton Scale)

If the company’s plant construction allows for the production on a thousand ton scale, the unit price per ton of fructose is \$1,800, the unit price per ton of catalyst 1 is \$10, the unit price per ton of solution 1 is \$900, the unit price per ton of solution 2 is \$1,100, and the unit price per ton of catalyst 2 is \$10. Fructose, solution 1 and solution 2 are directly part of the manufacturing process, and they take up the majority of material cost. However, even though catalyst 1 and catalyst 2 are not going to be transformed into other products through chemical reaction and can be used to expedite the reaction multiple times, there is also a cost occurs when reactivating these two catalysts. The company’s plan is to produce 300 ton for the first year, 600 ton for the second year and 1000 ton for the remaining three years. Their overall material costs are \$1,146,000, \$2,292,000, and \$3,820,000 respectively.

	Per ton	Year 0	Year 1 (3000t)	Year 2(6000t)	Year 3(10000t)	Year 4(10000t)	Year 5(10000t)
Material Cost			\$9,510,000	\$19,020,000	\$31,700,000	\$31,700,000	\$31,700,000
Fructose	\$1,700	\$0	\$5,100,000	\$10,200,000	\$17,000,000	\$17,000,000	\$17,000,000
Catalyst 1	\$10	\$0	\$30,000	\$60,000	\$100,000	\$100,000	\$100,000
Solution 1	\$650	\$0	\$1,950,000	\$3,900,000	\$6,500,000	\$6,500,000	\$6,500,000
Solution 2	\$800	\$0	\$2,400,000	\$4,800,000	\$8,000,000	\$8,000,000	\$8,000,000
Catalyst 2	\$10	\$0	\$30,000	\$60,000	\$100,000	\$100,000	\$100,000

Figure 18: Material Cost (Ten Thousand Ton Scale)

If the company’s plan construction allows for the production on a ten thousand ton scale, the unit price for fructose is \$1,700, the unit price for catalyst 1 is \$10, the unit price for solution 1 is \$650, the unit price for solution 2 is \$800, and the unit price for catalyst 2 is \$10. In comparison to producing on the thousand ton level, when producing on the ten thousand ton level, the unit price for each material, except for catalysts, drops due to marginal effect. Fructose, solution1 and solution 2 still take up the majority of the material cost. The plan is to produce 3000 ton for the first year, 6000 ton for the second year and 10000 ton for the remaining three years. Their overall material costs are \$9,510,000, \$19,020,000, and \$ 31,700,000 respectively.

Indirect Overhead is another crucial component of the manufacturing process. These may include cooling water, electricity, steam, and natural gas. These components are not part of the materials that directly produce FDCA, but without these utilities, the production objective will be impossible to achieve. Similar to the material cost, marginal effect is still at play depending on the production scale.

	Per ton	Year 0	Year1	Year2	Year3	Year4	Year5
Indirect Overhead			\$115,500	\$231,000	\$385,000	\$385,000	\$385,000
Cooling Water	\$40	\$0	\$12,000	\$24,000	\$40,000	\$40,000	\$40,000
Electricity	\$90	\$0	\$27,000	\$54,000	\$90,000	\$90,000	\$90,000
Steam	\$250	\$0	\$75,000	\$150,000	\$250,000	\$250,000	\$250,000
Natural Gas	\$5	\$0	\$1,500	\$3,000	\$5,000	\$5,000	\$5,000

Figure 19: Indirect Overhead Thousand Ton Scale

When producing on the one thousand level, the unit price for cooling water is \$40, the unit price for electricity is \$90, the unit price for steam is \$250 and the unit price for natural gas is \$5. Given the incremental addition of production in the first three

years, the overall indirect overheads are \$115,500, \$231,000, and \$385,000 respectively.

	Per ton	Year 0	Year 1	Year 2	Year 3	Year 4	Year 5
Indirect Overhead			\$885,000	\$1,770,000	\$2,950,000	\$2,950,000	\$2,950,000
Cooling Water	\$30	\$0	\$90,000	\$180,000	\$300,000	\$300,000	\$300,000
Electricity	\$60	\$0	\$180,000	\$360,000	\$600,000	\$600,000	\$600,000
Steam	\$200	\$0	\$600,000	\$1,200,000	\$2,000,000	\$2,000,000	\$2,000,000
Natural Gas	\$5	\$0	\$15,000	\$30,000	\$50,000	\$50,000	\$50,000

Figure 20: Indirect Overhead 20 (Ten Thousand Ton Scale)

When producing on the ten thousand level, the unit price for cooling water is \$30, the unit price for electricity is \$60, the unit price for steam is \$200, and the unit price for natural gas is \$5. Given the incremental addition of production in the first three years, the overall indirect overheads are \$885,000, \$1,770,000, and \$2,950,000 respectively.

Lastly, the incidental cost covers the depreciation of equipment and other costs that might occur during the manufacturing process that have not been considered yet. The estimated investment on equipment for the thousand ton scale is \$7,500,000 and considering the average depreciation rate of machinery for pharmaceutical factories is 10 years, the depreciation on equipment is \$750,000 every year. The estimated investment on equipment for the ten thousand ton scale is \$30,000,000 and using the same average depreciation rate of machinery for pharmaceutical factories, the depreciation on equipment per ton is \$3,000,000 every year. In addition, there are other costs that might accumulate during production such as managerial costs and other forms of costs that have not been considered yet. Comparing to another

on-going production task on a similar scale, the other costs per ton for the thousand ton scale is estimated to be \$800 per ton. The other costs per ton for the ten thousand ton scale is estimated to be \$80 per ton. Applying these estimations to the five-year-plan, the estimated costs for incidental costs were then calculated.

4.3.2 Sales

Although the market of FDCA is expected to be considerable, given that the development of FDCA is still on-going and major players in the market are still limiting their production to a “trial” quantity, the price of FDCA is expected to fluctuate for a certain amount as the industry unfolds. The price of FDCA will gradually decline as the production quantity continues to increase and the number of suppliers grows.

In the current stage, the suppliers of FDCA have set the price relatively high because the majority of FDCA purchased online or through other vendors is used for experimental purposes. This price is not comparable to when we actually use FDCA to produce PEF in placing of PET on an industrial scale.

Some of the forerunners, such as DuPont, in the pharmaceutical industry have started early production of FDCA on an industrial scale. Even though the price is still considerably higher than what we anticipate to be the acceptable price to challenge PTA, a compound that is used to produce PET which is a fuel-based polyester that we are trying to replace with PEF (a biomass-based polyester produced from FDCA), a noticeable drop in price has been detected. The current price of FDCA is

approximately \$33,000 per ton.

As the manufacturing of FDCA becomes increasingly mature, it is expected that the price continues to drop as the production of FDCA reaches one thousand ton scale and ten thousand ton scale. It is difficult to predict a precise price for FDCA at this point, yet it is possible to anticipate the price to land somewhere between \$20,000 to \$30,000 per ton for the thousand ton scale and \$5,000 to \$10,000 per ton for the ten thousand ton scale after factoring in its associated costs and availability. For the purpose of evaluating the profitability of FDCA, the average price of both scales were taken in order to produce the net sales and net present value.

4.3.3 Net Present Value

In order to quantify the net present value of both thousand ton scale and ten thousand ton scale, the function below was used to calculate and compare the net present value in a five year span:

$$\text{NPV} = (\text{Today's value of the expected cash flows}) - (\text{Today's value of invested cash})$$

Cash Flow			(\$8,700,000)	\$4,848,500	\$10,847,000	\$18,845,000	\$18,845,000	\$18,845,000
NPV (5 yrs.)	5%	\$52,304,566.09						
	15%	\$36,252,856.21						
	25%	\$25,663,561.60						

Figure 21: NPV (Thousand Ton Scale)

Cash Flow			(\$21,200,000)	\$8,465,000	\$20,330,000	\$36,150,000	\$36,150,000	\$36,150,000
NPV (5 yrs.)	5%	\$94,594,708.63						
	15%	\$63,944,300.93						
	25%	\$43,744,672.00						

Figure 22: NPV (Ten Thousand Ton Scale)

Different percentages of discount rate was used in order to make comparisons, and both NPVs are positive, indicating that the projected earnings generated by this investment exceeds the anticipated costs, and the manufacturing of FDCA is profitable.

4.4 Legal Analysis

The manufacturing of FDCA involves a specific design of production method that demands a precise and particular arrangement of equipment. This design is given by a research team based in Ningbo Institute of Materials Technology and Engineering. Due to the originality of such design and its potential profitability, this research team and its industrial design fall under the protection of Intellectual Property and the legality of the manufacturing process of FDCA needs to be resolved before moving forward.

Originally, Intellectual Property only protects “industrial property” such as patent, trademarks, and industrial designs. However, now the term “Intellectual Property” refers to a much wider definition and it helps enhance technology advancement in several ways:

(a) It provides a mechanism of handling infringement, piracy, and unauthorized use.

(b) It provides a pool of information to the general public since all forms of IP are published except in case of trade secrets. (Saha, 2016)

In the manufacturing industry, companies normally have their own distinctive

manufacturing process that takes advantage of the strength of the company. Even when presented with the same manufacturing objective, different companies might choose different routes to complete the same task. For example, in the case of manufacturing FDCA, companies that have more experience with glucose would be more inclined to choose that as the raw material to produce FDCA, while other companies might choose fructose instead. In addition, the chemical reaction process can also be entirely different based on the strength of the company. For instance, Avantium is known for their expertise in using enzyme as catalyst to help expedite the manufacturing process, while other companies would choose a more traditional path that uses metal such as platinum as catalysts. This minor difference would result in two completely different arrangements of equipment and the associated costs when fulfilling the same task.

Since this research team from Ningbo Institute of Materials Technology and Engineering proposed a specific production route for the company, there are two ways to avoid infringement in intellectual property when utilizing their design.

First, the company could simply purchase the manufacturing process and the research results from the research team for approximately \$1,200,000. This has been done multiple times with other projects and is the most straightforward way to employ the manufacturing method without illicit transgression.

Second, since the company has been working closely with the research team for several projects already and will most likely continue that collaboration in the future, they could also choose to compensate the effort and ingenuity of the research team

with forms of money, stocks or dividends. In return, the research team would allow the company to continue using their production method and help resolve other issues that might occur during manufacturing.

These are two potential approaches that the company could take under consideration to avoid intellectual property infringement. Whichever path the company ends up choosing to go with, the results of the research of producing FDCA on an industrial level will be used to their advantage so that they could move forward with the project. Deciding exactly which approach to take should also take into account whether the research team is required for the future or other business opportunities.

Chapter 5 -- Conclusion

This project showed that it is possible to produce FDCA on an industrial scale and the net present value would justify its production. Although some of the details still needs to be determined before officially starting to invest in the production of FDCA such as the exact production arrangement and how to purchase it from the research team, the outlook of FDCA is rather promising and could potentially generate a considerable amount of earnings for the company.

The results show:

- The unparalleled barrier properties of FDCA proposes great future in the making of PEF, which could potentially challenge the existing market of PET. The threats from PET's existing market and other competing companies should not deter dabbling into the production of FDCA as it is the trend to replace fossil-based material with renewable bio-based material going into the 21st century.
- Using fructose as the main raw material to produce FDCA through a series of reactions is industrially feasible, and the potential sales would be able to compensate the initial expenses and operating expenses while making profits for the company.
- There are at least two ways to utilize the results from the research team without infringing intellectual properties.

The production of FDCA was shown to be possible on an industrial scale and profitable on a five-year plan.

From completing this project, I learned that the courses I took during my time here at WPI can really facilitate me in my future work and help me understand

everything better from a business standpoint. Methods such as axiomatic design and financial analysis are great tools to break down complicated problems into simple ones and simplify the decision making process. I also learned that graduation only remarks the end of college and commences another phase of learning. While I was trying to complete this project, I was also learning different tools and technical terms to help me understand this project better, and it turned out that by the time I finished this project, I understood a lot more not only about this project, but also how manufacturing companies, especially chemical manufacturing companies, operate and make profits. This project was a great opportunity to use what I have learned throughout my college career and put them to practice. I have proven that I can use these methods to provide logic analysis and reasoning that eventually leads to a sound, evidence-supported decision. In the future, even though there is always more to learn and master, I envision great use of these methods and I know I can apply a lot of them when solving real world problems.

Chapter 6 -- Reference

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