HMF PRODUCTION USING AGRO-WASTE

By

ARLETH ADAMARIS ORTIZ

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Approved by:

Dr. Adrianna Brush

Department of Chemical and Environmental Engineering

Abstract

Annually, about 30% of the world's vegetable and fruit harvest is discarded as waste. Instead of allowing this abundant resource to degrade back into the environment, this agro-waste could instead produce 5-Hydroxymethylfurfural, or HMF. HMF is known to be a valuable, but expensive, intermediate compound found in the pharmaceuticals industry, in the creation of biofuels and solvents, and in building polymers, to name a few. The use of agro-waste will not only utilize its potential to create such an important chemical, but also minimize its presence in the environment.

The agro-waste is put through a five-step process: a subcritical water hydrolysis reactor, simulated moving bed chromatography, byproduct purification, glucose to fructose conversion, and finally, fructose to HMF conversion. Annually, the project utilizes about 169,000 metric tons of agro-waste and converts that into about 8,270 metric tons of HMF. HMF profit alone is around $380 million; however, when combined with byproduct sales, the plant yields a total yearly profit of about $1.05 billion.

Although the plant creates such a high profit, further research is advised to minimize water and utility usage and to find several resources for agro-waste so as not to completely deplete one source immediately.

CHEE 443

Senior Design Project

HMF Production Using Agro-Waste

Group 17

Bryce Long

Brendan Greene

Arleth Ortiz

Sam Herschler

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Summary

The primary goal of this plant is to deliver a steady supply of 5-hydromethylfurfural (HMF) to the market utilizing the abundance of agricultural waste as the raw material needed. The main criteria and optimization goals for the plant were to minimize water and energy usage. As of now, the plant produces over 8,200 metric tons of HMF a year with a total sales value of over 1 billion dollars a year. The plant intakes 169,000 metric tons of agriculture waste a year and consumes 105 million gallons of water a year. The amount of water used is roughly the demanded needed of a food processing plant. There is uncertainty behind how the HMF market would react to a large increase in supply but that is beyond the scope of the plant. Other sources of uncertainty include the logistics and transportation of getting agricultural waste to the plant were not accounted for. Another was the use of simulated moving bed chromatography and the complexities associated with it. A great deal of assumptions and simplifications were made, coupled with the fact that SMBC is a vital part of plant, casted some uncertainty on the units which relied on it.

Overview of Contributions

Bryce Long

- Summary
- Introduction
- Written description of SWH
- Equipment Description of SWH

Sam Herschler

- Legal guidelines for environmental impact, help with LCA
- Written description of Glucose to Fructose Unit
- Equipment description of Glucose to Fructose Unit
- Global, Social, Cultural Impact(s)
- General editing and formatting
- References

Brendan Greene

- Final Economic Analysis
- Utility Table and description
- Written description of SMBC
- Written description of Byproduct Purification
- Equipment Description of SMBC
- Equipment Description of Byproduct Purification
- Conclusion

Arleth Ortiz

- Quantitative Block Flow Diagrams
- Process Flow Diagrams
- Equipment Tables
- Stream Tables
- Written Description of Fructose to HMF
- Equipment Description, Rationale, and Optimization of Fructose to HMF
- HAZOP Analysis
- Life Cycle Assessment
- References

Table of Contents:

Introduction

During the earliest stages of plant design, the goal was to deliver a chemical to the open market that could help the industry progress away from fossil-based chemicals and to more sustainable and eco-friendlier alternatives. At first, we looked at 2,5-Dimethylfuran (DMF) to be that chemical – a potential biofuel which compares to that of gasoline and could be derived from another compound, 5-Hydroxymethylfurfural (HMF). However, we soon switched to the goal of mass producing 5-Hydroxymethylfurfural after more research showed the vast potential of HMF as a versatile biomass-derived chemical[1]. In terms of being a sustainable and eco-friendly alternative, HMF could be synthesized from fructose, glucose, cellulose, biomass, and lignocellulosic materials. HMF is often referred to as "sleeping giant" due to the anticipated enormous market potential of HMF and its derivatives[38].

Once we had finalized our choice on HMF, we switched to deciding what our raw material would be. One of the first considerations was to simply buy bulk fructose as it was the most straight forward method to produce HMF via dehydration of fructose. Aside from this, there was also the option of buying/converting glucose to fructose. We shortly turned away from these options however and opted to utilize biomass and lignocellulosic materials to produce HMF. Using these waste feedstocks meant that they weren't competitive with food industries and reduced the energy and financial as opposed to fructose/glucose[1]. Coupled with this was the fact that roughly 20-30% of global fruit/vegetable are discarded as waste during post-harvest handling, according to the Food and Agriculture Organization (FAO), helped us make the decision to use agricultural waste for our raw material source for HMF production.

Agriculture waste is mostly composed of cellulose, hemi-cellulose, and lignin of different percentages depending on the agro-waste. These organic polymers when subjected to hydrolysis

will yield a variety of reduced sugars, most important fructose and glucose. Typical large scale and industrial hydrolysis involves the use of strong acids and bases along with pretreatments of various enzymes and alkalines to promote the breakdown of the lignocellulosic material. We found that these methods had high costs associated with them and produce contaminants which must be separated in post-treatment, resulting in non-coverable costs[2]. Therefore, subcritical water hydrolysis (SWH) technology was chosen early on to counter-act some of these drawbacks.

SWH used only water to breakdown our agro-waste, allowing our plant to reduce its environmental footprint and reduce post-treatment complexity. Water is considered the ideal green solvent with its nontoxicity and low cost. This technology could be applied to a wide variety of agro-wastes: it has lower costs, ease of use, and has reduced reaction times compared to conventional hydrolysis[3]. However, due to the severe process conditions, industrial application of this technology suffers from various challenges. Namely, high temperatures and pressures required would put tough requirements on process components such as feed pumps. In addition, these conditions posed higher safety requirements for plant design. In short, most work on SWH has so far been carried out in lab- or bench-scale and high investment cost is a considerable hurdle for commercialization[4]. This was apparent at the time of selecting this technology, and still is at the writing of this report. Despite these issues, the ability to process different agro-waste and produce similar reduced sugars aligned with our main goal for the plant.

With a SWH reactor able to process a variety of agro-waste, we chose pecan shells to model our plant off of due to their large agricultural presence in Arizona coupled with a relevant lab scale research using SWH on shell dust[4]. However, this choice in agro-waste wouldn’t be the final choice in future due to how accepting of SWH technology to different agro-waste. Rather,

choosing pecan shell dust would serve as an example waste to simulate how generic plant waste would be processed in the plant. In other words, the choice of agriculture waste would change the types of reduced sugars we yield from hydrolysis, but would also produce some amount of glucose, fructose, and HMF.

Due to SWH indiscriminately breaking down the biopolymers of our agro-waste, the product stream would contain not only water, glucose, and HMF but also other reduced sugars such as arabinose and xylose. Separation and isolation of glucose and HMF from the product stream led us to use Simulated Moving Bed Chromatography (SMBC). This technology would let us separate each product and byproduct from the post-reactor product stream with high purities. In the same vein as SWH, an SMBC unit had never been fully scaled to and built in industrial setting, but had been extensively researched for decades, allowing us to create an accurate upscaled design with costs and feasibility data available. This had been a large hurdle the team faced during last semester and into a good portion of this year, but after its completion gave way for the development of a byproduct purification unit and subsequent water recycling. In fact, the majority of this semester's work revolved the finalization of the SMBC unit, followed by byproduct purification, and the incorporation of recycle water into the SWH unit which will be described below.

Process Description

Subcritical Water Hydrolysis

There are five main objectives that this unit must accomplish:

1. Deliver a residue-free product stream to SMBC at a set temperature.
2. Supply adequate water as desorbent for the two SMBC units.
3. Maintain subcritical water conditions.
4. Maximize energy recovery.
5. Minimize water usage.

There were 4 material inputs for this unit: the WATERIN, RECYCLE, PECDUST, and COOLING stream. The WATERIN stream represents the plant's main water intake that comes from outside the plant. This stream first encounters the preheater HX-102, then is mixed (S-1) with the recycled stream (S-2) inside M-102. The combined stream (S-3) proceeds to the water pressurizer P-101 to prepare water for subcritical conditions. Next, the pressurized stream (S-4) enters the main heat exchanger HX-103 to produce subcritical water. Pressurization with P-101 before heating the water past 100C ensured that no phase change occurred. After heat, the stream (S-5) enters the reactor (R-101). This reactor is pre-loaded with suspended pecan dust and the water in S-5 continuously runs through the material. The PECDUST stream depicts the ground-up pecan shell dust being loaded into the SWH reactor during downtime. A heat jacket is built into the reactor walls to maintain subcritical water conditions (HEATJACK). At the end of the reactor is a mesh-screen to capture the pecan residue and carbon-build up to prevent it from traveling downstream (S-101). The mesh-screen is periodically changed/removed during semi-batch operations, shown as RESIDUE in the PFD. The now residue-free product stream (S-7)

travels to HX-104 where it is cooled down, then even further in HX-105. Keep in mind that this stream is still pressurized, so cooling it down to less than 100C ensures that no phase change occurred when S-9 entered the depressurization valve (V-101) - bring it back to atmospheric pressures. After V-101, the product stream (S-10) enters a final heat exchanger (HX-106) to further cool down to the ideal temperature demanded of SMBC. The TOSMB stream is the SWH's final product stream, carrying all the reduced sugars, furfural, and HMF, which makes its way to the SMBC portion of the plant.

The RECYCLE stream was a combination of all byproduct waste streams and the final effluent from both SMBC units. This stream contained trace amounts of reduced sugars (>1%) that weren't completely removed from byproduct purification. The incorporation of this stream helped significantly reduce the amount of water used by the plant overall. The RECYCLE stream was a combination of vapor and liquid, so it was cooled by running it through HX-101 to ensure a completely liquid stream (S-2) before being mixed with S-1 in M-102. Finally, the COOLING stream is another water intake from outside the plant, used as the desorbent in the two SMBC processes of the plant. Similar to the WATERIN, this stream needed to be heated to a specific temperature which was accomplished with HX-107.

Outside of input and outlet streams, this process used serval close looped streams to maximize energy recovery. This is primarily due to the high temperatures associated with subcritical water, heating for SMBC desorbent, and cooling demand of the recycle stream. The inner loop consisting of streams L-1, L-2, & L-3 served as the cooling water loop responsible for the final heating of the water before entering R-101 using HX-103. The cooling water stream (L-2) would enter HX-104, being heated up by cooling down the product steam leaving the reactor (S-8). The now heated water utility stream (L-3) then encounters the electric heater H-101 which

increases the temperature enough to fulfill the heating needed to raise S-4 to subcritical conditions (L-1).

The next loop consists of streams D-1 and D-2 which goes through heat exchangers HX-102 and HX-106. These streams use more utility water in a close looped heat exchanger network to ensure that S-10 is cooled to the specific temperature needed for SMBC using HX-106. The excess heat of D-2 is used in HX-102 to increase the temperature of WATERIN stream in the form of a preheater. The cooled utility water D-1 then completes the loop by returning to HX-106.

The streams for the final loop were P-1 through P-9 and were used to recover energy from the recycle stream and transfer it to the COOLING stream. This is because the two SMBC units in the plant need water at specific temperature for their processes. This objective was done using HX-101 where the RECYCLE stream was cooled by P-8. Stream P-9 then carries the latent energy to be mixed with P-3 inside M-101. P-3 was another energy recovery stream which came from cooling off the product stream in HX-105. After mixing in M-101 the new stream (P-4) enters HX-107, heating up the COOLING stream to fulfill the temperature requirements needed for the absorbents. The remaining energy in the utility water (P-5) is then sent to a series of cooling towers (CT-101, CT-102, & CT-103) for further cooling before leaving as stream P-1. To complete the loops, this stream enters a flow separating block (SP-101) to deliver optimal flow to HX-101 and HX-105.

Simulated Moving Bed Chromatography

The main goals of the simulated moving bed chromatography (SMBC) portion of the plant are to separate the products from SWH and purify the water. The flow from SWH is too

large to pass through 1 SMBC unit so it is split between 10 rows of SMBC units (only 1 row is shown in Figure #3 for simplicity). In each row there are 5 units, SMB-201A/B to SMB-205A/B. The products separated out are furfural, HMF, arabinose, xylose, and glucose, in that order. The waste streams from each unit are recycled back into the plant and the now separated streams are sent to the byproduct purification unit.

Byproduct Unit

The main goals of the byproduct purification portion of the plant are to further purify reduced sugars and recover more water to be recycled. For arabinose, glucose and xylose, flash drums F-601 to F-603 are used to boil off the water. For HMF, distillation column D-601 is used to reach the required 95% purity. Lastly membrane filtration, shown in Figure #5, was chosen to purify furfural due to the azeotrope present between furfural and water. The final products are sent to holding tanks and the recovered water is recycled back into the plant.

Glucose to Fructose Unit

There are two primary objectives of this unit. The first objective of this unit is to convert the glucose produced from the Simulated Moving Bed Chromatography Unit to fructose by utilizing a tubular reactor filled with Ca-Al catalysts. The second objective is this unit is to separate the mixture of glucose, fructose, and water from the outlet of the tubular reactor by using a second SMBC unit, recycle the water in use, and purify the remaining glucose. The second SMBC unit separates the glucose and fructose into two outlet streams. One outlet stream has a majority sugar composition of fructose, while the other outlet stream has a majority sugar composition of glucose. The majority fructose and water stream is sent to the Fructose to HMF Unit, while the majority glucose and water stream is sent to a separator unit, where the glucose

and water are separated. The pure water stream from the flash separator outlet is then recycled back into the plant, and the purified glucose is then sold as a byproduct.

First, the tubular reactor R-301 receives the feed stream of glucose and water from the SMBC Unit. After reacting at 45^{o} Celsius at a pressure of 1 bar with the aid of Ca-Al catalysts, the outlet stream of R-301 is composed of glucose, fructose, and water. This stream then enters an 8-column SMBC unit, SMB 301 A/B. SMB 301 separates the fructose and glucose at a temperature of 80^{o} Celsius, using a desorbent stream into the bottom of the first SMBC column to aid in the separation of glucose and fructose. SMB 301A/B and has two outlet streams composed of separated sugars and water; the product and the raffinate. The product stream, with a majority sugar composition of fructose, is fed to the Fructose to HMF Unit. The raffinate stream, with a majority sugar composition of glucose, is fed to a separator unit, S-301. S-301 separates the water from the majority glucose sugar at a pressure of 1 bar, resulting in two outlet streams. The first outlet stream is composed of pure water and is sent back to the Subcritical Water Hydrolysis Unit as a recycle stream. The second outlet stream is 99.7% pure glucose, which is collected as a byproduct for later sale.

Fructose to HMF Unit

The main objective of this portion of the process is to take the fructose from the Glucose to Fructose conversion process and convert it into HMF.

To begin, the fructose is taken and mixed with water at a 30% w/v ratio in VSS-401. In VSS-402, DMC and HCl are combined; DMC is entering at a rate that is three times the volume of the aqueous fructose solution while HCl is added to a final concentration of 0.23 M. The mixture from VSS-401 is mixed together with the contents of VSS-402 before being sent to

pump P-501, where it is pressurized from 1 bar to 20 bar. This pressurized flow is then sent to plug flow reactor R-401, where the contents react with each other at 200C. The pressurized hot contents exit the reactor and enter heat exchanger HXT-501, where cooling water of 25C cools the mixture down to 40C. Pressure relief valve V-401 depressurizes the mixture back down to 1 bar. Before entering extractor E-401, the mixture has two phases: an organic phase (DMC and HMF) and an aqueous phase (water and HCl). The purpose of the extractor is to separate the phases, sending the organic phase to an evaporator and the aqueous phase to a flash drum for further processing. Evaporator EV-401 heats the DMC and HMF to 101C, recycling most of the DMC back to the extractor while outputting the final HMF product. The aqueous phase that is sent to flash drum F-401 is heated to 100C, outputting extra HMF while sending the remaining liquid out to be dealt with as waste.

Quantitative Block Flow Diagram:

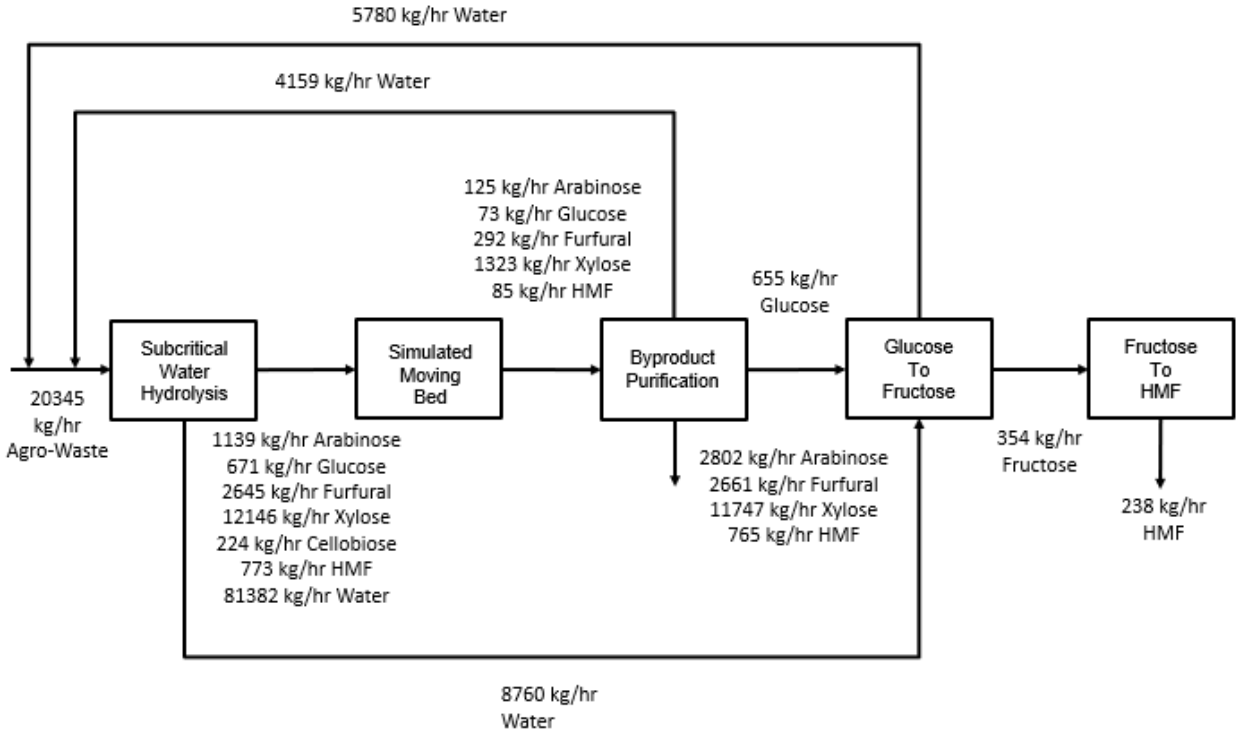

Figure #1: Quantitative Block Flow Diagram of Entire Process

Process Flow Diagrams

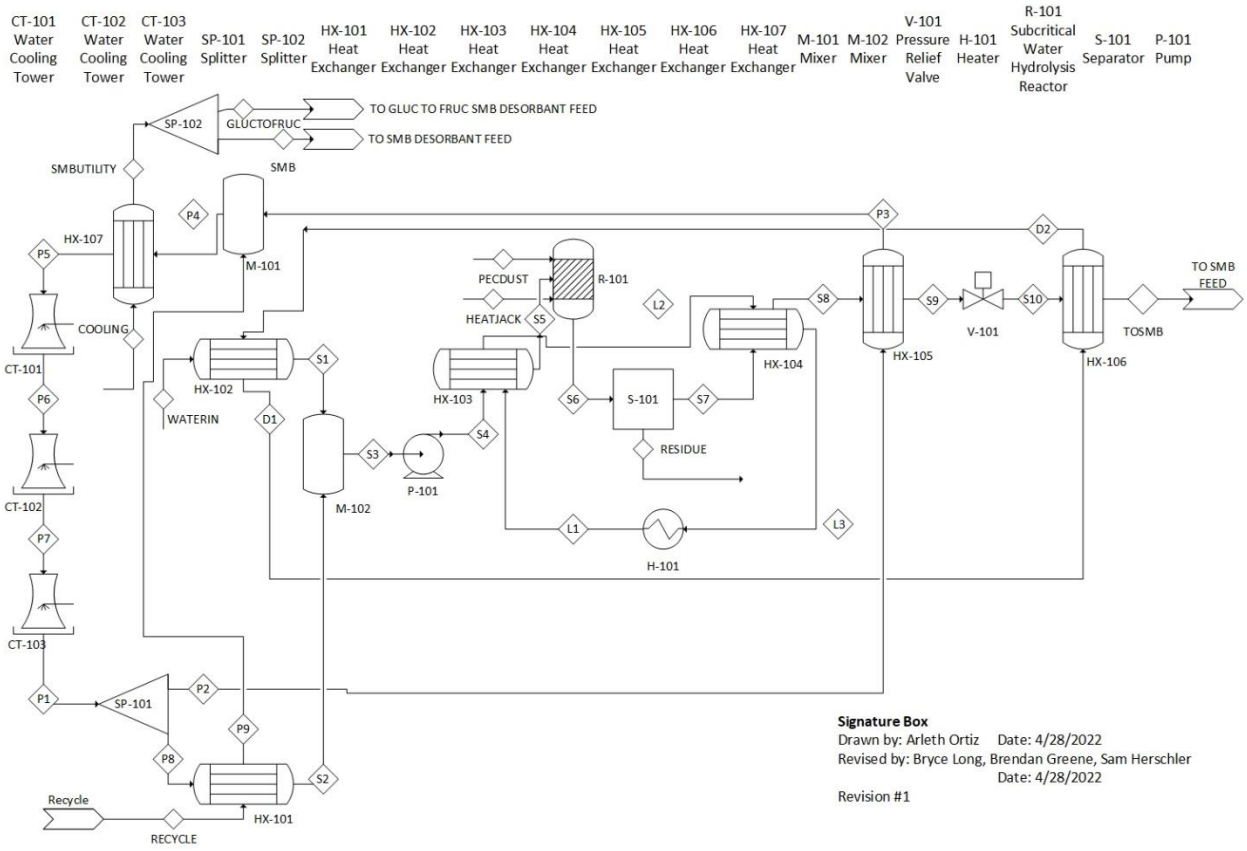

Figure #2: PFD of First Step in Process—Subcritical Water Hydrolysis

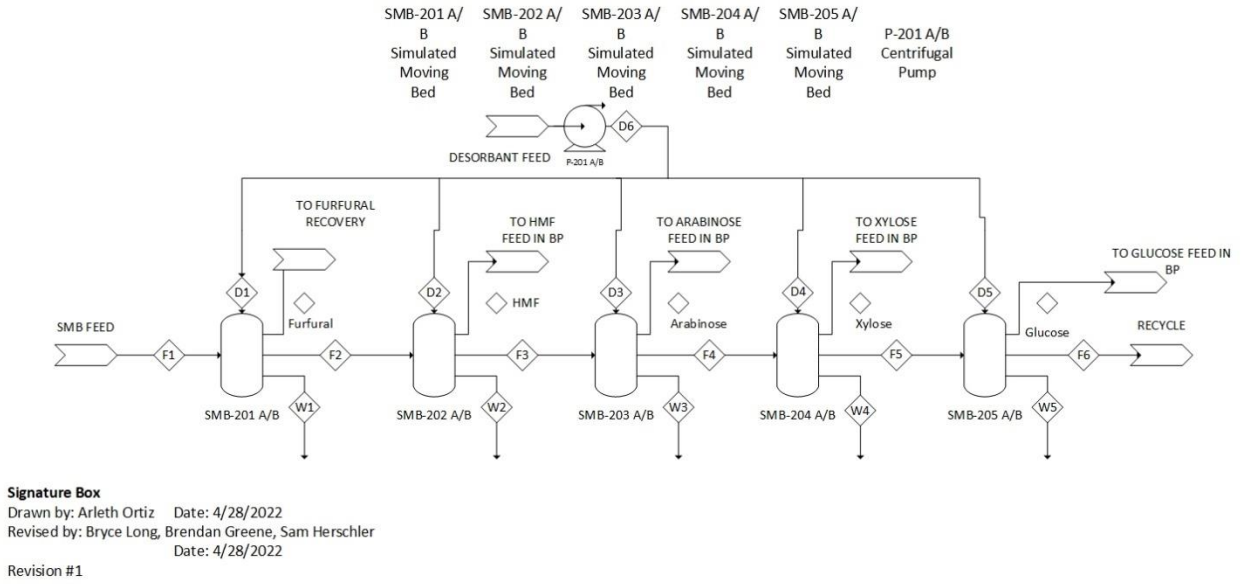

Figure #3: PFD of Second Step in Process—Simulated Moving Bed Chromatography

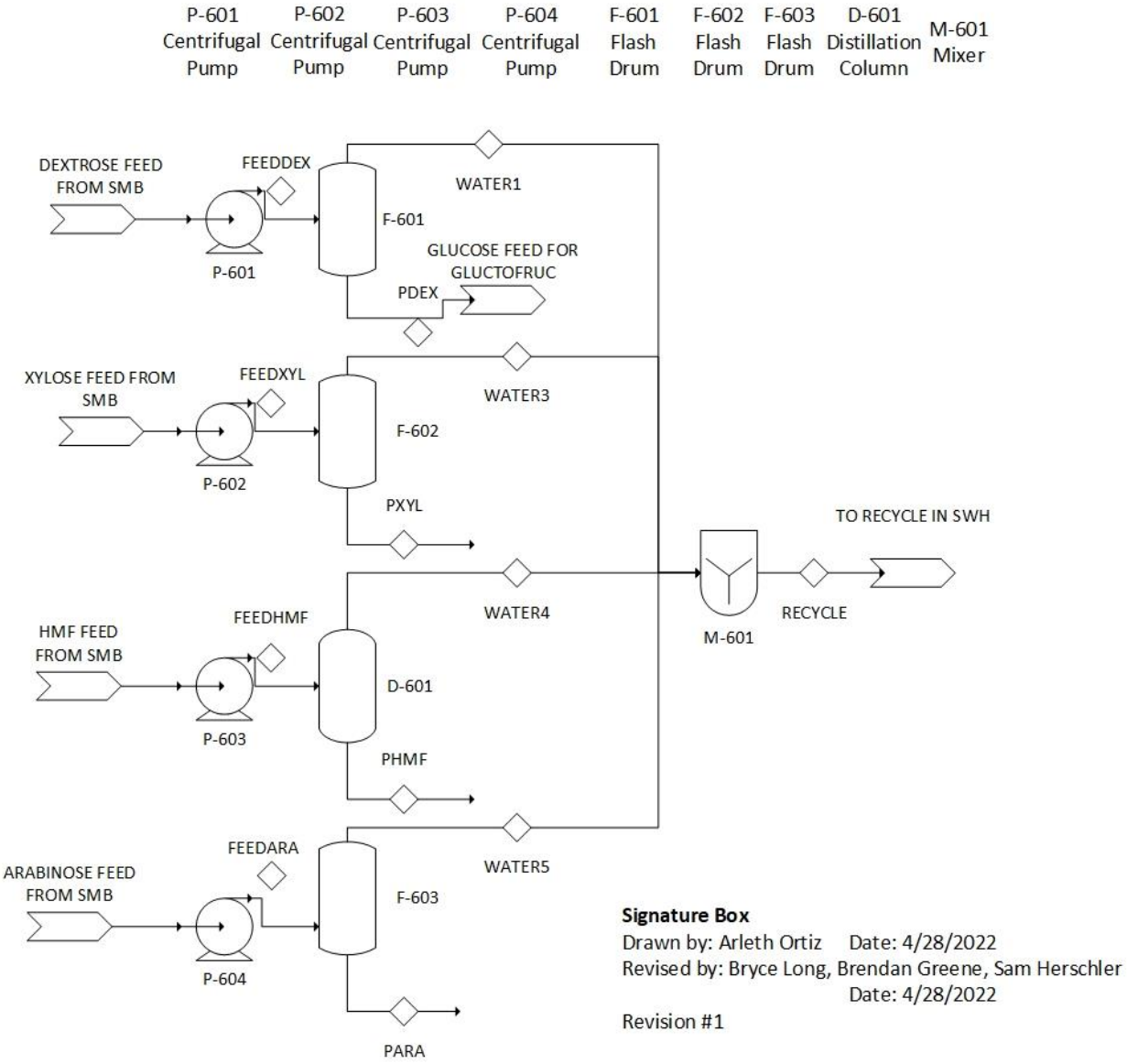

Figure #4: PFD of Third Step in Process—Byproduct Purification

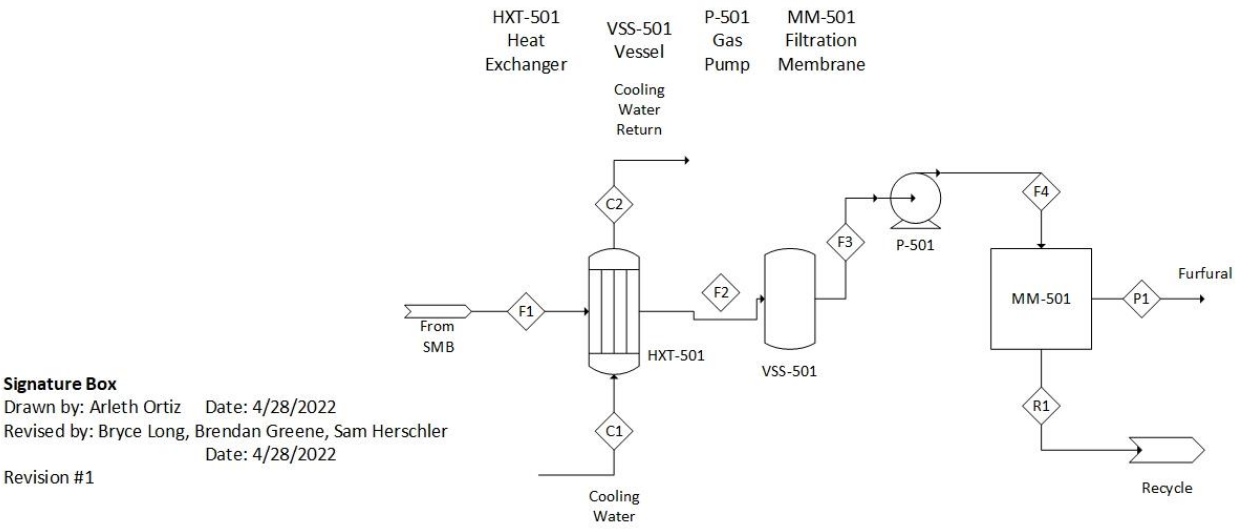

Figure #5: PFD of an Addition to the Third Step in Process—Furfural Recovery

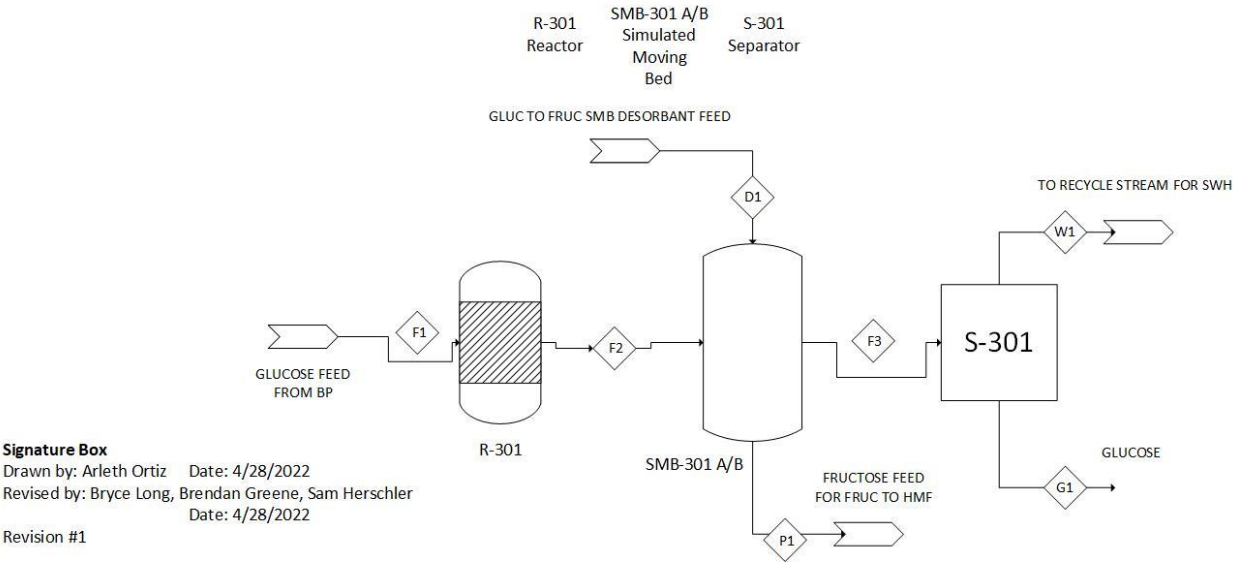

Figure #6: PFD of Fourth Step in Process—Glucose to Fructose Conversion

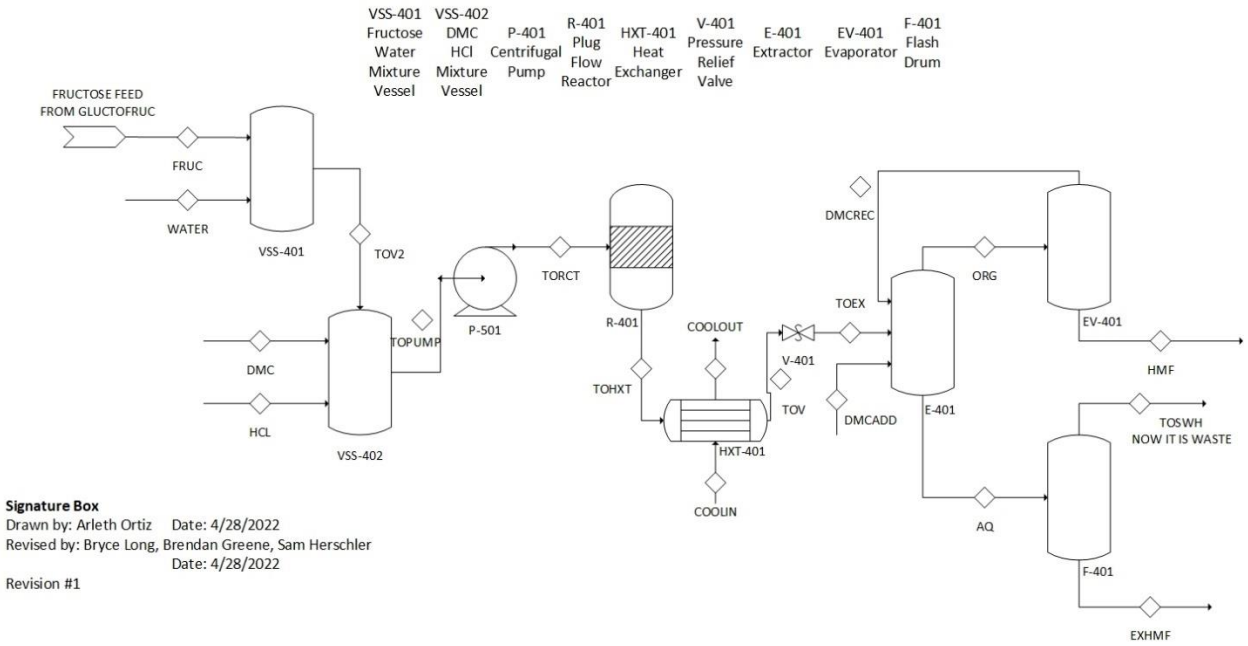

Figure #7: PFD of Final Step in Process—Fructose to HMF Conversion

Equipment Tables

To see equipment tables, go to Table #8 in the Appendices.

Stream Tables

To see the stream tables, go to Table #9-15 in the Appendices.

Utility Table

A table summarizing the plant's annual energy and cooling water usage is provided below.

Cooling water	77,608,883	gal/yr
Energy	35,867.82	kW

Table #1: Annual Utilities

The total cooling water usage for the plant is over 77 million gallons of water per year which makes up over 3/4th of the total water usage for the plant; the majority of which is used to cool off the recycled water stream in the cooling towers. The total energy usage of the plant is over 35,000 kW, the largest portion of the energy usage comes from the xylose flash unit which requires over 24,000 kW. To minimize this high energy usage an alternative method should be chosen. If the energy required was minimized cooling water would also be saved due to the lower temperature of the recycled water.

Equipment Description, Rationale, and Optimizations

Subcritical Water Hydrolysis Unit

Prior to optimization, the SWH unit did not incorporate the recycled water stream, nor the heating requirements needed for absorbent flow for SMBC. Because of this, the process used only one closed-cooling loop. However, the incorporation of the recycle waste-water stream brought along some crucial changes to the unit. More specifically, how to maximize energy recovery and minimize water usage. Just with the introduction of the recycle waste-water stream drastically reduced our water demand, which was drawn from outside the plant, by ~50%. However, the recycle stream needed to be cooled and fully converted to liquid before it was mixed together with the fresh water prior to pre-heating. This was done by creating a closed heat exchanger network which would siphon off energy from the recycle stream and hot product stream in the SWH unit and use it to heat up absorbent streams for SMBC. This achieved the goal of fully phase changing the recycle stream to liquid so it could be mixed and supply adequate water for the two SMBC units. Despite this, the shear amount of energy present in the recycle stream entering the SWH unit caused us to look to large industrial methods of cooling a high volume of water. Thus, we elected to use cooling towers to remove the excess heat after all

primary goals were achieved. We calculated that we needed 3 cooling towers to successfully reduce the temperature of water to an ideal condition. Unfortunately, there were unavoidable water losses using cooling towers, but we were unable to find a better alternative that could perform as well.

Heat Exchangers (HX-103 & HX-104)

Besides the recycle stream, more closed-loop heat exchangers were added to maximize the energy recovery effort and minimize energy usage. Heat exchangers HX-103 and HX-104 were the first additions this semester to help cool down the hot product stream leaving the SWH reactor and heat the water just before entering the reactor. These closed loop exchangers also relied on an inline electric heater (H-101).

Inline Electric Heater (H-101)

The chief piece of equipment that required the most energy in the unit was the inline electric heater (H-101), which was incorporated into the first heat exchanger loop to make up for unavoidable energy losses. The main method of reducing the energy needed was by adding more preheating to the water in streams S-1 through S-4. This is because the higher the temperature the reaction water entering HX-103 (S-4), meant the lower amount of work H-101 needed to do as its built into the HX-103 and HX-104 loop.

Heat Exchangers (HX-102 & HX-106)

As stated before, a big optimization scheme was to raise the temperature of reaction water before entering HX-103. To help with this, HX-102 served as the first preheater the freshwater intake stream encountered when entering the unit. Stream D-2 acted as the hot utility stream which would transfer energy into the water heading towards R-101 (S-1). The now cooled

D-1 utility stream would travel to HX-106 to siphon off energy from the hot product stream and return to HX-102. By doing this, it helped meet the goal of delivering products to SMBC at the specific temperature of 70C and also minimize energy needed of H-101.

Heat Exchanger (HX-101)

The incorporation of the recycled wastewater resulting from the byproduct and SMBC units helped us reduce water usage but also created a new problem. The problem was that the conditions of the recycled stream were both vapor and liquid at around 100C. To properly mix it with the freshwater intake needed for the reactor, HX-101 was used to cool down the recycle stream enough so that only phase present in stream S-2 was liquid. Keeping the phase of S-2 and S-1 liquid was important because once they were mixed into S-3, they would be pressurized to 300 bars. If S-3 contained any portion of vapor phase, significant damage could be done to the pump (P-101) via cavitation.

Heat Exchangers (HX-105 & HX-107)

Another goal of the SWH unit was to provide fresh water at 70C to the two SMBC processes later in the plant. Due to the amount of cooling and heating energy available in the SWH unit, it was decided that the goal would be accomplished by siphoning off energy (P-3) from the hot product stream (S-8) with HX-105 and cooling utility stream (P-2). This helps reduce the product stream temperature and use stream P-3 to mix (M-101) with P-9. This stream was the utility stream that was heated in HX-101 using the hot recycle stream. The combined stream (P-4) flowed into HX-107 as a hot utility which heated up the fresh water to 70C, which was needed for SMB desorbent.

Cooling Towers (CT-101, 102, & 103)

Due to the fact the recycle stream was partially vapor and liquid, and the quantity of it resulted in a large amount of excess heat energy available to the SWH unit. Unfortunately, only so much of it could be used to preheat the freshwater intake by mixing S-2 with S-1 without resulting in vapor before the pump (P-101). This excess energy from the recycle stream took the form of stream P-9 which was sent to mix with P-3 as previously described. However, despite running P-4 through HX-107, P-5 remained a considerably hot liquid (~80C). Without wanting to bring in more fresh water which would increase our plant's water usage, we instead employed a series of three cooling towers to lower the water temperature to roughly ~25C as stream P-1. This temperature was needed to adequately cool the recycle inlet stream (P-8) using HX-101 and sent the excess cooling water (P-2) to HX-106 with a flow separator (SP-101). In summary, by using cooling towers this kept the water utility loop closed outside of the natural water loss associated with using cooling towers.

Subcritical Water Hydrolysis Reactor (R-101)

The SWH reactor (R-101) didn't undergo large changes with it came to optimization. Because it was a yield reactor with the yield numbers coming from associated reference paper[4], the entire SWH unit was built around satisfying the conditions required for subcritical water conditions (220C and 300 bars). The only relevant changes were changing the original water to biomass mass ratio of 15/1 described in the paper and set to 4/1 by reducing the amount of fresh water drawn from outside the plant. This was done because the ratio ensured that water could never be a limiting reactant in the paper, but the actual ratio was never optimized to minimize water usage. By looking at another reference papers[2] which delved into the feasibility of upscaling a SWH reactor from lab scale, this papers water to biomass ratio was used. The last change on the reactor was to incorporate a heat jacket to ensure constant temperature throughout

the reactor. Due to the complexity of the plant, we didn't have to resources to fully research this heat jacket, so instead we did a basic energy calculation to determine heat duty using ASPEN Plus.

Pressure Relief Valve (V-101)

With a goal of delivering 70 C and ~1 bar product stream to the SMBC unit, a pressure relief valve was needed as the product stream immediately leaving the reactor was still 300 bars. However, due to the fact that it was also 220C, the hot product stream was sent through a series of heat exchangers (HX-104 & HX-105) so that the stream entering the pressure relief valve (V-101) would be around ~95 C. The reason it was designed this way was to ensure that product stream didn't undergo phase change and remained a liquid to reduce complexity of the process. V-101 would change S-9 from 300 to ~1 bar.

Simulated Moving Bed Chromatography

Simulated Moving Bed Chromatography (SMB-201-5A/B)

SMBC is a complex process that expands on batch chromatography. SMBC works by simulating a moving stationary phase through complex valve switching and timing. This allows for an almost infinite column length to be achieved in a compact space. SMBC is more efficient compared to batch chromatography as it can be run continuously and uses the stationary phase more efficiently. It is also highly efficient at separation, capable of achieving purities of over 99.5%.

This separation technique was chosen for the plant mainly due to its ability to be run continuously. Due to the complexity of SMBC most of the calculations are simplified, and no valve times or valve switching order was calculated. Before the construction of this plant can be

considered a more in-depth calculation should be done on this unit to determine the final details such as valve times, valve positions, and column sizes.

Pumps (P-201-9A/B)

These centrifugal pumps are responsible for pumping the desorbent through each SMB unit row. The flow rate for these pumps is 74 gallons per minute and the power requirement for the pump motors is 7.3 horsepower.

Byproduct Purification

Arabinose Flash Drum (F-603)

The arabinose flash drum was modeled in ASPEN and had a final volume of 1050L which was based on a residence time of 17.5 minutes. The heat duty of the drum was determined to be 3080 kW.

Xylose Flash Drum (F-602)

The xylose flash drum was modeled in ASPEN and had a final volume of 14045 L which was based on a residence time of 17.5 minutes. The heat duty of the drum was determined to be 24381 kW. This is our most energy intensive unit in the entire plant and would likely require further optimization to get the energy usage down.

Glucose Flash Drum (F-601)

The glucose flash drum was modeled in ASPEN and had a final volume of 936L which was based on a residence time of 17.5 minutes. The heat duty of the drum was determined to be 1606 kW. Not all the water was recovered from this stream as the glucose is converted into fructose later in the plant and water is required.

HMF Distillation Column (D-601)

The HMF distillation column contains 30 trays and has a reflux ratio of 0.1. The total heating duty of the column is 2202 kW, and the cooling duty is 2087 kW. This is what is required to reach a 95% purity of HMF.

Pumps (P-601-4A/B)

These pumps are responsible for moving the liquid product from SMBC to the byproduct purification. The sizing of these pumps is based on flowrate which range from 17 to 210 gallons per minute (23). The motors for these pumps range from 1 to 20hp and were sized with the same reference (23). The chosen material of construction for these pumps was 316 stainless steel as they would not come into contact with any highly corrosive chemicals.

Glucose to Fructose

Prior to optimization, R-301 ran in a batch configuration of 4 reactors with volumes of 18599.157 L each, utilizing the catalyst Zirconium UiO-66 for glucose isomerization to fructose in a solvent of 1-propanol. This configuration was based on laboratory experiments done by Matheus Dorneles de Mello and Michael Tsapatsis in their work *Selective Glucose-to-Fructose Isomerization over Modified Zirconium UiO-66 in Alcohol Media*. While this batch configuration resulted in fructose yield of 56%, it was difficult to model and run successfully in ASPEN software due to Zirconium UiO-66 not being available in ASPEN as a usable catalyst, and a lack of available rate data from the publication in order to estimate a reaction constant. In addition to the reactions in R-301 being difficult to model and having a lack of available rate data, the separation of fructose and glucose was left unfinished, with eventual separation of glucose and fructose being assumed.

The conversion of glucose to fructose in R-301 was optimized by having a continuous isomerization of glucose to fructose, with R-301 being a tubular, fixed-bed reactor instead of a series of batch reactors. In addition, the tubular reactor utilized the catalyst $Ca_3AlO_{4.5}$ instead of Zirconium UiO-66. At a reaction temperature of 45^o Celsius, the optimized, continuous flow conversion of glucose to Fructose in R-301 had a 54% yield and was substantially easier to model in Aspen. This conversion scheme was based on laboratory experiments performed by Maria Ventura, Jamie Mazario, and Marcelo E. Domine in their work *Isomerization of Glucose-to-Fructose in Water over a Continuous Flow Reactor using Ca-Al Oxide as Heterogeneous Catalyst*.

R-301

The final volume of R-301 was calculated to be 7596.8275 L, and the mass of $Ca_3AlO_{4.5}$ in the reactor was calculated to be 1636.95 kilograms. From *Isomerization of Glucose-to-Fructose in Water over a Continuous Flow Reactor using Ca-Al Oxide as Heterogeneous Catalyst*, the lab-scale reactor volume was not given. Instead, the final volume of R-301 was estimated with the incoming flowrate from the SMBC Unit. Using the flowrate from the SMBC Unit, 3.038731 m^3/hr, the residence time of the reactor on an experimental scale was estimated by taking the lab-scale volumetric flowrate, 2ml/hr, converting it into a mass flowrate of .2g/hr, and then dividing the mass flowrate into the lab scale reactor by the mass of $Ca_3AlO_{4.5}$ in the reactor, .5 to get a residence time estimate of 2.5 hours. By assuming the residence time of the reactor stayed constant, the final volume of R-301 was calculated to be 7596.825 L. Using the fructose yield value of 54% from the literature, the fructose output from R-301 was calculated to be 1958.25 mol/hr, or 358.5812 kg/hr. Tables displaying calculations of these values are available in supplemental data provided in the final calculations for this project.

The optimization of the separation of glucose and fructose was done utilizing SMB-301 A/B; an eight-column SMBC process. Since the previous separation process was confined to a black box problem, this section of optimization was largely done from scratch in order to simply achieve the separation of glucose and fructose. Ultimately, a second SMBC unit was utilized for the separation of glucose and fructose due to the success of the first SMBC unit in the process, SMB-201-5A/B, when separating glucose from other reduced sugars in the Subcritical Water Hydrolysis unit of the experiment. Further cementing the usage of a second SMBC unit was the lack of research and papers supporting alternative methods of separating glucose and fructose besides SMBC. At a reaction temperature of 80^{o} Celsius, SMB-301 was able to produce two outlet streams: the product and raffinate streams, respectively. The product stream had a yield of 99.7% of the fructose entering SMB-301A/B, while the raffinate stream had a yield of 99.7% of the glucose entering SMB-301A/B. This separation scheme was based on optimization research done for an eight-column SMB unit by York A. Beste, Mark Lisso, Gunter Wozny, and Wolfgang Arlt in their work *Optimization of simulated moving bed plants with low efficient stationary phases: separation of fructose and glucose.*

SMB-301 A/B

For SMB-301 A/B, the required desorbent for the successful separation of was found to be water after a translation of *Simulierte Gegenstrom-chromatographie* by Petra Deckert und Wolfgang Arlt. This paper was one of the references listed in *Optimization of simulated moving bed plants with low efficient stationary phases: separation of fructose and glucose* and used the same eight column setup. The desorbant flowrate was calculated utilizing the desorbant consumption constant provided in the literature, M, and the final column sizes remained

unchanged from the model described in the literature utilized. Tables displaying calculations of these values are available in supplemental data provided in the final calculations for this project.

From SMB-301 A/B, the product stream is sent to the Fructose-HMF Unit. The raffinate stream, however, is sent to S-301, a separator unit. S-301 is a generic separator unit in ASPEN, used for the purpose of separating the large amount of glucose in the raffinate stream from the water in the raffinate stream. This was implemented to improve overall water use efficiency by having the water utilized in SMB-301A/B be recycled back into the Subcritical Water Hydrolysis Unit; the unit operation that makes use of the most waste in the entire plant. With the glucose separated from the water, 99.7% pure glucose was collected and sold as a byproduct to further increase the profitability of the plant.

S-301

Due to time constraints, a specific method for separation and experimental data regarding separating glucose from water could not be gathered or analyzed. Thus, S-301 is not operating based on experimental data, and the value for the outlet flows of glucose and water were input in an ASPEN program based on what was required for an optimal water recycle stream. The flowrate of water from the S-301 outlet was calculated to be 5775 kg/hr, and the flowrate of glucose was calculated to be 301.356 kg/hr. In addition, fructose that wasn't fully separated in SMB-301 A/B had an outlet flow of 1.05816 kg/hr. This left the glucose outlet with a purity of 99.64%.

Fructose to HMF

It must be noted that all pieces of equipment, besides VSS-401, are made with monel steel[13]. Monel steel has been shown to be one of the few cheaper alternatives to other metals that can withstand HCl at multiple concentrations. Because the process handles HCl at 0.23 M, regular stainless steel will begin to encounter corrosion sooner than it would with monel steel. Nickel alloys have also been shown to be resistant to HCl corrosion, but no feasible material of construction number could be found in *Plant Design and Economics for Chemical Engineers* to be used in the calculations; therefore, monel steel was used.

The volumes were determined by calculating the minimum required volume from residence time and volumetric flow rates and the operating factor of 65%

This Fructose to HMF part of the process has been based on the lab experiment done by Sayed et al., therefore, each piece of equipment has been included to replicate said experiment.

Vessel (VSS-401)

The inclusion of a vessel is for the simple reason of welcoming in the fructose and water streams and mixing them together, as done in the lab experiment. With Aspen numbers, the volume was determined to be around 330L; however, this was increased to 500 L so as to not be operating at full capacity.

Vessel (VSS-402)

The inclusion of another vessel, again, is for the simple reason of mixing in the DMC and HCl streams and mixing them together, as done in the lab experiment. With Aspen numbers, the

volume was determined to be around 330 L; however, this was increased to 500 L so as to not be operating at full capacity.

Pump (P-501)

A centrifugal pump was chosen to pressurize the fluid from 1 bar to 20 bar. The pump handles 22.2 gal/min and requires only a mere 3.58 hp to operate at these conditions; the pricing and size for this pump, found in the Final Calculations, used the 6/10 rule in comparison to a table found in *Plant Design and Economics for Chemical Engineers.*

Reactor (R-401)

A plug flow reactor is used to react fructose, water, DMC, and HCl at 200C in order to produce the HMF product. The volume was found to be around 330 L, big enough to hold all the contents with a residence time of just one min.

Heat Exchanger (HXT-501)

In the lab experiment, it dictated that some sort of unit was used to cool the effluent from the reactor from 200C to 40C. It was decided that a shell and tube heat exchanger could perform this task best. As per Heuristic 55 (Seider et al), the tube side, or the "hazardous fluid" side, was used for the effluent while the shell side, or the "clean fluid" side was used for the cooling water. The heat exchanger area was maximized to 62 ft^2 in order to decrease water usage, as that is one of the bigger issues that the plant faces.

Pressure Relief Valve (V-401)

The purpose of including a pressure relief valve was to depressurize the mixture from 20 bar to 1 bar as to make it easier for downstream unit ops to handle and to also decrease the potential price of having to design the unit ops to handle 20 bar.

Extractor (E-401)

Due to the reaction in the reactor, two phases were created: an organic and aqueous phase. On a lab scale, a simple phase-separation vessel was used; on the industrial scale, an extractor was one of the only successful pieces of equipment that was found that could successfully separate the phases. The extractor was upsized to 200 L, as about 142 L were coming out of the reactor.

Evaporator (EV-401)

On the lab scale, a rotary evaporator was used to best separate the organic phase holding DMC and HMF from each other; an evaporator was found to produce the same results on the industrial scale. Around 100 L is entering the evaporator; therefore, the volume was upsized to 200 L as to not have a potential overflow.

Flash Drum (F-401)

The flash drum is the only piece of equipment not found in the lab experiment, the reason for this being that there was a belief that there was more HMF product contained in the aqueous phase. Therefore, this piece of equipment was included to fully optimize the production of HMF. A flash drum was then added to take this aqueous phase, run at a high temperature in hopes to have one exit stream to be waste while the other to contain more HMF. This thought process proved to be successful, as this is exactly what happened.

Safety Issues

Section 1: HAZOP Analysis

Project Name: HMF Production Using Agro-Waste	Date: 3/16/23	Page 1 of 1
Process Equipment (PFD #): R-101	**Name of Individual Doing Review: Bryce Long**	
Section: Subcritical Water Hydrolysis	Reference Drawing:	

Study Node	**Process Parameters**	**Deviations (Guide Words)**	**Possible Causes**	**Possible Consequences**	**Action Required**
Subcritical Water Hydrolysis Semi-Batch Reactor	Flow	No Flow	L - Broken high pressure water pump upstream. L – Clogged heat exchanger up or downstream.	Product not made, heat/energy wasted at exchangers, possible melt down or rupture of pipes upstream.	Shutdown of main water source, water heaters and removal of stationary phase in reactor. Repair/cleaning of upstream piping.
		Less Flow	L – Insoluble buildup within upstream heat exchanger. M – Stationary phase in reactor was improperly changed, restricting flow. M – Buildup of stationary residue inside reactor. M - Malfunctioning pump, partially blocked line. M – Piping downstream is has restricting flow.	Product production hindered. Unwanted temperature increases	Diversion of water away from reactor, removal/cleaning of buildup/residue, add detergent into water stream for specific time. Manuel cleaning may be needed.
		More Flow	L – Upstream water pump is malfunctioning H - Stationary phase inside reactor is nearly depleted or improperly changed.	Further unwanted degradation of product may occur	Diversion of water from primary pump to backup pump. Direct water away from primary reactor and to secondary reactor which is on standby.

Temperature	Too Low	L – An unwanted endothermic reaction is taking place inside reactor. L – High pressure pump is failing to pressurize water to set point, resulting in phase change in water when heating is applied. M – Upstream heat exchanger is failing to heat cold water to specific temperature. This can be due to build up within the exchanger or failure of inline water heater between up and downstream heat exchanger.	Unwanted byproducts are being made that will contaminate product stream, Product production hindered; more unreacted material left in reactor.	Analyze composition of water recycle stream for trace chemicals upstream. Divert flow to backup high pressure water pump. Repair. Divert flow to backup heat exchanger. Clean/repair if needed. Same for inline heater
	Too High	L – An unwanted exothermic reaction is taking place inside reactor. M - Upstream heat exchanger provides too much heating to cold water before entering reactor. This could be due to failure of inline water heater between up and downstream heat exchanger.	Possible runaway reaction could occur inside reactor. Resulting temp. increase could raise pressure, leading to catastrophic failure of reactor wall, leading to high pressure/temp water steam escaping. Chucks of steel debris could be sent outwards in all directions at high speeds. Melting of pipes and heat exchanger could also occur. Product could degrade further.	Switch from hot water circulating in reactor heat jacket to cold water. If temperature cannot be stabilized, divert water from reactor. Open pressure relief valves and rapidly dump remaining fluid from reactor. Send water to standby reactor. If the problem is with the heat exchangers, switch to backups, if possible, otherwise complete system shutdown
Pressure	Too Low	L - Malfunctioning high pressure water pump upstream. L – Reactor walls are compromised. M – Improperly sealed flanges, joints, or compromised piping	Unwanted phase change of water may occur. Product production hindered, gas escapes into environment.	Diversion of water from primary pump to backup pump. Diversion of water from reactor/piping and to standby reactor. Depressurize and repair.

	Too High	L – Gaseous buildup in reactor due to unwanted side reaction. L - Malfunctioning high pressure water pump upstream. L – Overheating of water upstream heat exchanger before flowing into reactor. M – Stationary phase in reactor was improperly changed, leading to pressure buildup. M – Piping downstream is either clogged or restricting flow.	Catastrophic failure of reactor wall, leading to high pressure/temp water steam escaping. Chucks of steel debris could be sent outwards in all directions at high speeds. In the case of piping, rupture could also occur at joints, seals, and other areas of weakness	Open pressure relief valves at areas close to high pressure source. If pressure isn't controlled this way, heaters and the primary water source are to be cut off. Complete system shutdown. If the reactor is compromised, redirect to standby reactor

Table #2: HAZOP Analysis of Subcritical Water Hydrolysis Reactor, R-101

Project Name: HMF Production Using Agro-Waste	Date: 3/16/23	Page 1 of 1
Process Equipment (PFD #): SMB-201-5 & SMB-301	**Name of Individual Doing Review: Brendan Greene**	
Section: Simulated Moving Bed	Reference Drawing:	

Study Node	**Process Parameters**	**Deviations (Guide Words)**	**Possible Causes**	**Possible Consequences**	**Action Required**
SMB	Flow	No Flow	L – Clogged rotary valve, broken pump, incorrectly packed bed	Air gaps will form which could damage pumps in process as well as downstream.	Shut down SMB Unit and transfer feed to back up unit.
		Less Flow	L – pump malfunction, incorrect switching time, debris in packed bed	Could result in air gaps which will damage pumps in unit as well as downstream.	Check to see if pumps are working correctly, if not transfer flow to back up unit.
		More Flow	L – pump malfunction, decomposition of packed bed, increased pressure drops	Could result in excess ware of packed bed stationary phase and add stress on pumps in process and downstream.	Could result in excess ware of packed bed stationary phase and add stress on pumps in process and downstream.
	Temperature	Too Low	L– malfunction with upstream heat exchanger	Separation will not be as efficient, increased wear on stationary phase.	Separation will not be as efficient, increased wear on stationary phase.
		Too High	L – malfunction with upstream heat exchanger	Gas could form inside column, causing excess ware on pumps and valves in process and downstream.	If temperature rises above 100C for an extended period of time, divert flow to back up column and check unit components for ware from steam build up.

Pressure	Too Low	L – decrease in flow rate to column, leak in column	If resulting from leak could result in spill which is a hazard for workers.	Check units for leaks, if there is a leak, transfer work to back up unit and immediately work on repairs.
	Too High	L – increase in flowrate to column	Column could fail structurally resulting in an explosion.	Include a pressure relief valve on each unit to ensure pressure does not build up to excess.
Composition	Too Low	L – poor yield in SWH unit upstream, incorrect switching time, increased flow from desorbent feed	SMB will not run as efficiently decreasing yield of sugars and downstream yields.	Unit should still be able to run at decreased efficiency. Check upstream SWH for yield problems.
		L – incorrect switching time, decreased flow from desorbent feed	SMB will not run as efficiently, and product streams could become contaminated resulting in decreased yield and side reactions downstream.	Increase desorbent flow rate. If desorbent pump is malfunctioning, then divert feed to back up unit.

Table #3: HAZOP Analysis of Simulated Moving Beds, SMB-201-5 A/B & SMB-301

Project Name: HMF Production Using Agro-Waste	Date: 3/16/23	Page 1 of 1
Process Equipment (PFD #): R-401	**Name of Individual Doing Review: Arleth Ortiz**	
Section: Fructose to HMF	Reference Drawing:	

Study Node	**Process Parameters**	**Deviations (Guide Words)**	**Possible Causes**	**Possible Consequences**	**Action Required**
Reactor	Flow	No Flow	L- Pump broken, pipeline backed up with influents, formation of humins	Extractor and evaporator will dry.	Shut down of all unit ops
		Less Flow	L- Not enough supply of influents, incorrect flows inputted, pump backed up or not working well	Unit ops downstream will dry up	Check if pumps are working properly, influents on correct measurements. If not- use backup pumps while working to fix other
		More Flow	M- Incorrect supply of influents, more of something than other	Can overflow unit ops downstream, heater will not have enough time to heat all liquid and cause separation errors	Slow down influent rates to prevent unit ops flooding
	Temperature	Too Low	H-temperature controller not working.	Could potentially yield less HMF and decrease fructose conversion. Less desired products	Stop process. Can leave liquids in reactor and investigate cause of temperature malfunction.
		Too High	H-temperature controller not working	Could potentially yield less HMF and decrease fructose conversion. Less desired products. Burn fructose faster than it could react	Stop process. Can leave liquids in reactor and investigate cause of temperature malfunction
	Pressure	Too Low	M-pressure regulator not working.	Could potentially yield less HMF and decrease fructose conversion. Less desired products	Stop process. Drain liquids to side vessel and investigate cause of pressure malfunction.

		Too High	H-pressure regulator not working	Can decrease desired product yield and overwhelm downstream unit ops	Stop process. Drain liquids to side vessel and investigate cause of pressure malfunction
	Level	No Flow	L- Pump broken, pipeline backed up with influents, formation of humins	Extractor and evaporator will dry	Shut down of all unit ops
		Less Flow	L-Broken pump or clogged pipes/entrance to reactor due to sugar byproducts	Yield less desired products as reaction relies on certain molar concentrations and inputs	Start backup pumps while stopping broken ones. Drain liquid to another vessel and clean out reactor
		More Flow	M-Clogged outlet	Will eventually flood reactor and prevent any more reactions. Pressure will build	Drain liquid to another vessel and clean out reactor.

Table #4: HAZOP Analysis of Fructose to HMF Reactor, R-401

Table #2 highlights all the hazards that come with operating R-101, the subcritical water hydrolysis reactor. It summarizes how either flow, temperature, or pressure can affect the unit and all downstream unit ops if there is none, too high, or too low of the operating parameters. The flow issues could deal with malfunctions of the pumps or clogged pipelines, which can hinder overall production. Temperature issues can come from unwanted reactions occurring or the heat exchanger providing too much water to the streams that are entering the reactor; unwanted byproducts and other reactions can occur. Pressure issues arise from malfunctioning pieces of equipment or other gas buildups from reactions inside the reactor, which can cause catastrophic consequences to both the reactor and plant as this piece of equipment is highly pressurized, potentially causing injury to workers.

Table #3 highlights all the hazards that come with operating the SMB units. It summarizes how either flow, temperature, pressure, or composition can affect the unit and all downstream unit ops if there is none, too high, or too low of the operating parameters. The flow issues could deal with malfunctions of the pumps or clogged pipelines, which can hinder the design of the SMB columns overall. Temperature issues can come from heat exchanger malfunctions and prevent proper separation. Pressure issues arise from flow rate fluctuations, which can cause leakage in the columns. Compositions issues come from flowrate fluctuations and incorrect switching times, which can decrease the yield coming out of the SMB units.

Table #4 highlights all the hazards that come with operating R-401, the fructose to HMF reactor. It summarizes how either flow, temperature, or pressure can affect the unit and all downstream unit ops if there is none, too high, or too low of the operating parameters. The flow issues could deal with malfunctions of the pumps or clogged pipelines, which can dry up downstream unit ops. Temperature issues can come from controller malfunctions and can cause

less HMF yield. Pressure issues arise from malfunctioning regulators, which can cause less HMF yield. Finally, level issues stem from broken or clogged pieces of equipment that will either dry up downstream unit ops, yield less products, or flood the reactor.

Environmental Impact Statement

Section 1: Legalities

For this project, the three main categories of environmental impact we will be examining are water use, CO2 emissions, and land usage. However, legal statutes for environmental impact largely revolve around water use and land use rather than CO2 emissions. For water use, legal statutes in Arizona are largely based on the water resource utilized. For this plant, the Central Arizona Project (CAP) will be the sole water source. Usage of the CAP is organized and dictated by federal and statutes. Federally, the CAP and its subsidiaries are organized under Title 43-Public lands, Chapter 35, of the U.S Code. The original statutes and limitations for usage of the CAP were signed into law as the *Colorado River Basin Project Act of 1968.* Title 43, Chapter 5 states that "water from the Central Arizona Project shall not be made available directly or indirectly for the irrigation of lands not having a recent irrigation history as determined by the Secretary, except in the case of Indian lands, national wildlife refuges, and, with the approval of the Secretary, State-administered wildlife management areas" (Title 43-Public Lands, 1524 (a) U.S Code). While usage of the CAP is limited to tribal and federal lands in principle, contracts with private industries can be made with the approval of the U.S Secretary of the Interior: "Irrigation and municipal and industrial water supply under the Central Arizona Project within the State of Arizona may, in the event the Secretary determines that it is necessary to effect repayment, be pursuant to master contracts with organizations which have power to levy assessments against all taxable real property within their boundaries… the United States shall, if

the Secretary determines such action is desirable to facilitate carrying out the provisions of this chapter, have the right to require that it be a party to such contracts or that contracts subsidiary to the master contracts be entered into between the United States and any user," (Title 43-Public Lands, 1524, (b) U.S Code).

CAP land and water usage for industries is permitted through a two to three-phase application process. The initial application details the use of the land and water for a proposed project and is reviewed by the governing board of the Central Arizona Water Conservation District (CAWCD) (Central Arizona Project AZ, Land Use). When the proposed project is deemed acceptable, applicants must fill out a required form. The type of required form(s) is based on the type of project proposed. For short term projects such as research, design survey work, and environmental/cultural survey work, applicants must fill out either a Right of Entry Notice or a Special Use Permit (Central Arizona Project AZ, Land Use). Long-term projects, such as the proposed HMF plant, are categorized based on levels of ground disturbance, and require a Land-Use-License (LUL), permitted by the CAWCD (Central Arizona Project AZ, Land Use). Once the LUL is secured, long-term projects must additionally fill out a Consent Document. The Consent Document is permitted upon approval of the LUL and acknowledges improvements and ground-disturbing activities that take place on and off CAP land and ensures protection of CAP facilities (Central Arizona Project AZ, Land Use).

Under Title 43 of the U.S code, the CAP is a federal project. While under local jurisdiction by Arizona authorities, the CAP must ultimately answer to and adapt to any new federal statutes, and land decisions made by CAWCD must abide by statutes enforced by the United States Bureau of Reclamation (Central Arizona Project AZ, Land Use). Currently, the most prominent environmental statute the CAP must abide by is *Colorado River Drought Contingency*

Plan Authorization Act, which was signed into law in 2019. The *Colorado River Drought Contingency Plan Authorization Act* consists of two contingency plans developed to combat an ongoing drought that has lowered the level of the Colorado River Basin to 39% of its original capacity, having previously been at 95% capacity in the year 2000 (Colorado River Drought Conditions, Office of Congressional and Legislative Affairs). In Arizona, this drought is evident in the declining water level of Lake Mead, which supplies water to the CAP. The plans are divided amongst the different basins of the Colorado River, with the CAP occupying the lower basin. The corresponding Lower Basin Drought Contingency Plan (DCP). The DCP implemented measures designed for regions in the Lower basin to share water resources from the Colorado River, and by extension the CAP, to reduce the drainage of Lake Mead. Combined with the upper basin DCP, the utilization of the DCP reduces the risk of Lake Mead water levels dipping below the critical threshold of 1025 feet by 2026 from a 43% risk to an 8% risk (Central Arizona Project, Drought Contingency Plan: Arizona Implementation).

Section 2: Life Cycle Assessment (LCA)

The following figures categorize the impacts made by the more detrimental pieces of equipment found in each individual section of the process, with a replicate of the SMB unit as both the second step of the process and the glucose to fructose conversion step utilize such units.

It is assumed that the LCA summarizes the impacts made where the pieces of equipment have been created for the process.

Category	Weight	Units
Land Use	3.37E+05	Items
Climate Change	1.35E+05	kg
Photochemical Ozone Creation	257	kg
Aquatic Ecotoxicity	3.14E+05	Items
Aquatic Eutrophication	83	kg

Figure #8: Summarization of LCA done on Subcritical Water Hydrolysis Reactor, R-101

The land use is the heaviest weighted when it comes to R-101. The reactor is rather large, with a weight of 191441 pounds and a volume 43675 L, so it comes to no surprise that this unit will have repercussions on the environment. This perhaps alludes to the land that was used to gather and collect the materials needed to make the reactor. The next heaviest weighted category is aquatic ecotoxicity. This can be paired with aquatic eutrophication as both deal with damage done to the aquatic ecosystem. These impacts could perhaps be caused by the emissions emitted when creating the reactor. Climate change is the next heavier category, dealing with emissions that have damaged the air, water, and land around the plant that has created the reactor. Finally, the photochemical ozone creation may have been caused when the reactor was in production, the plant expelling volatile organic compounds out into the air and increased ground level ozone that may affect human health (M.E. Jenkin et al.).

Category	Weight	Units
Land Use	1.86E+06	Items
Climate Change	7.49E+05	kg
Photochemical Ozone Creation	1421	kg
Aquatic Ecotoxicity	1.74E+06	Items
Aquatic Eutrophication	458	kg
Water	7.29E+06	m3

Figure #9: Summarization of LCA done on Simulated Moving Bed, SMB-201 A/B

One overall LCA was done for both the Simulated Moving Bed process and the Glucose to Conversion process as both units are practically the same.

The water is the heaviest category, in terms of numbers. In the OpenLCA program, it states that it has taken water from river water and to and from a turbine; therefore, building this SMB had enough impact from withdrawing all that water from nearby resources. The land use is the next heaviest weighted. The SMB is rather large, with a weight of 477116 kg and a volume 7068 L, so it comes to no surprise that this unit will have repercussions on the environment. This alludes to the land that was used to gather and collect the materials needed to make the reactor. The next heaviest weighted category is aquatic ecotoxicity. This can be paired with aquatic eutrophication as both deal with damage done to the aquatic ecosystem. These impacts could perhaps be caused by the emissions emitted when creating the units. Finally, the photochemical ozone creation may have been caused when the reactor was in production, the plant expelling volatile organic compounds out into the air and increased ground level ozone that may affect human health (M.E. Jenkin et al.).

Category	Weight	Units
Land Use	499	Items
Climate Change	201	kg
Aquatic Ecotoxicity	465	Items
Water	1952	m3

Figure #10: Summarization of LCA done on Byproduct Purification Distillation Column, D-601

The water is the heaviest category, in terms of numbers. In the OpenLCA program, it states that it has taken water from river water and to and from a turbine; therefore, building this distillation column had enough impact from withdrawing all that water from nearby resources. The land use is the next heaviest weighted. This alludes to the fact that land was used to gather and collect the materials needed to make the distillation column. The next heaviest weighted category is aquatic ecotoxicity. These impacts could perhaps be caused by the emissions emitted when creating the column into any nearby waterways. Climate change is the next heavier category, dealing with emissions that have damaged the air, water, and land around the plant that has created the column.

Category	Weight	Units
Land Use	23	Items
Climate Change	9	kg
Aquatic Ecotoxicity	21	Items
Water	89	m3

Figure #11: Summarization of LCA done on Fructose to HMF Reactor, R-401

The water is the heaviest category, in terms of numbers. In the OpenLCA program, it states that it has taken water from river water and to and from a turbine; therefore, building this reactor had enough of an impact from withdrawing all that water from nearby resources. The land use is the next heaviest weighted. This alludes to the fact that land was used to gather and collect the materials needed to make the reactor. The next heaviest weighted category is aquatic ecotoxicity. These impacts could perhaps be caused by the emissions emitted when creating the column into any nearby waterways. Climate change is the next heavier category, dealing with emissions that have damaged the air, water, and land around the plant that has created the reactor.

Global, social, cultural, public health and welfare impacts

From a global perspective, the novel synthesis of HMF through agricultural waste can effectively reduce pollutant emissions from internal combustion processes utilized in widespread technology such as cars. This is due to HMF serving as the core basis for the creation of the eco-friendly biofuel, 2,5-dimethylfuran (DMF). Derived from HMF, DMF possesses attractive qualities for internal combustion, such as high boiling point (92-94^{o} C), a low water solubility of .26%, and an octane number of 119 (Chapter 5: Biofuel Production From Biomass: Toward

Sustainable Development, 85). A fuel's octane number represents the stability of a fuel in the combustion cylinder of an engine, with more stable fuels having a lower propensity for spontaneous combustion. A higher octane number correlates to a lower rate of spontaneous combustion and higher efficiency of the fuel in question (U.S. Energy Information Association, "What is Octane?"). The octane number of DMF is considerably higher than that of commonly utilized E10 (10% ethanol content) gasoline, which has a typical maximum octane number of 93 for "premium grade" fuel (U.S. Energy Information Association, "What is Octane?"). Therefore, DMF is a much more efficient fuel for internal combustion engines than E10 gasoline.

This efficiency advantage over E10 gasoline pairs well with the reduction in greenhouse gas emissions such as CO2 in vehicles with direct injection spark ignition (DISI) engines, due to DMF's spark sensitivity. Regarding DISI engines, spark ignition timing "significantly affects the combustion process, which determines the fuel economy, torque output and emissions performance" of vehicles with spark-ignition engines (Ritchie, Et al., 72). Related to spark timing, a fuel's "spark sensitivity" is a measurement of how variations in spark timing during ignition impacts the combustion of a fuel. An examination of indicated specific CO2 emissions (is CO2) produced by ethanol, DMF, gasoline, butanol, and methanol in DISI engine defined that "the increase in isCO2 is a function of the spark sensitivity of each fuel" (Ritchie, Et al., 80). The results of the examination displayed that "the CO2 increase with gasoline is 19.4%, whereas with ethanol and DMF it is 5.6% and 10.7%, respectively" (Fuel, Daniel). While having more CO2 emissions than ethanol, DMF nonetheless produced fewer CO2 emissions than gasoline, demonstrating its potential as an eco-friendly biofuel. The notable advantages that DMF possesses, namely efficiency and reduced CO2 emissions, can only be utilized once it is

synthesized through HMF. Through the synthesis of HMF, via agricultural waste as an input, production of a promising biofuel can be buoyed.

Regarding the synthesis of HMF, the current synthesis process involves the usage of 105,000,000 gallons of water per year for the conversion of agricultural waste to glucose, assuming high efficiency and proper optimization Given that the HMF synthesis plant will operate in Eloy, Arizona, it is paramount to address how the usage of 105,000,000 gallons of water per year will impact the surrounding communities in Eloy, native tribes in Arizona, and communities in Arizona as a whole. At the time of publication, the state of Arizona is currently in the midst of a Tier 1 water shortage. Defined by the Central Arizona Project (CAP, Colorado River Shortage), water shortage tiers are determined by the elevation of the water line in Lake Mead, a reservoir that collects water from the Colorado River (CAP, Colorado River Shortage). The Colorado River itself is the largest water resource for Arizona, providing approximately 36% of the state's water supply (Arizona Water Facts, Arizona's Water Supplies). A Tier 1 water shortage is indicated by water elevation levels dropping below 1075 feet in depth. As a result of the water shortage, the CAP reduced its water delivery by 512,000 AF, or acre-feet, of water. This course of action to preserve and water levels in Lake Mead will "be borne by Central Arizona Project () water users," resulting in "less available Colorado River water for central Arizona agricultural users" (Central Arizona Project).

The CAP supplies water to Maricopa, Pinal, and Pima counties, with the plant site in Eloy being situated in Pinal County. Therefore, the proposed HMF plant and the city of Eloy are both subject to the CAP's reduction in the water supply. Historically, Eloy's economy has been based on agriculture. While the city's economy has diversified in recent years, agribusiness is still a prominent economic tentpole, as Eloy occupies "part of the Santa Cruz Basin, which is one

of Arizona's most fertile agricultural areas, with more than 100,000 irrigable acres" (ELOY PDF). With the CAP's water reductions in mind, Eloy must now grapple with a generally reduced water supply from the CAP; reductions that overwhelmingly impact agricultural enterprises. Considering the importance of Eloy's agriculture due to the proposed HMF production plant's intake of pecan shells from Eloy pecan farms, the task of reducing water use in HMF production is a vital undertaking to ensure sustainability for Eloy. While optimization of water use through the use of recycle streams has been successful in relegating net water usage to levels similar to the food production industry, it is still in the best interest of the proposed plant and the community of Eloy for water use to be further reduced, in order to avoid excess strain on an already troubled water distribution system.

A further consequence of increased strain on the Colorado River basin through this proposed plant's water uptake is the impact it will have on Native American communities in Arizona. From its legal inception in 1968, the CAP has always fulfilled the role of water provider for Native American communities across the state. Of 22 federally recognized tribes in the state of Arizona, 14 tribes have either partially or fully resolved water rights disputes. Of those 14 tribes, a large number of them receive or have received large portions of their water through the CAP (Central Arizona Project, tribal Water Rights). The 2004 Arizona Water Settlements Act allocated 67,300 acre-feet of CAP water to address any remaining water rights claims from the tribes. Of that amount, 33,107 acre-feet is currently available for resolving future settlements. In total, 46% of all CAP water is allocated to Native American communities in Arizona, meaning that potential risks to the CAP due to the ongoing drought and increased drainage from the proposed plant will have an outsized impact on Native American communities. And while there is an ongoing drought, some tribes have curbed their use of CAP water, instead relying on other

tribes through the sharing of surplus water. While this conservation of the CAP's water supply is admirable, the implications for some tribes are ethically troubling. For example, "Jay Weiner, a lawyer who represents tribes in water rights settlements, said it would be unjust to continue to rely heavily on tribes when they haven't had access to the water as long as states in the basin" (Associated Press, State of Unease: Colorado basin tribes without water rights).

Final Economic Analysis

Table #5 contains all the equipment prices for the plant. All the reactors and vessels were cost based on weight of the unit op using “Plant Design and Economics for Chemical Engineers” (23). The SMB units were priced from Xie et al (36). The pumps and motors were priced off graphs from various sources depending on the required flowrate and motor power (23)(19). A further explanation for costing and sizing can be found in the attached calculation sheet.

Equipment	Cost	Total # in Plant	Total Cost
R-101	$ 7,697,222	3	$ 23,091,666
R-301	$ 36,914	2	$ 73,828
R-401	$ 28,692	2	$ 57,384
HXT-101	$ 2,413,006	2	$ 4,826,011
HXT-102	$ 349,597	2	$ 699,195
HXT-103	$ 17,865,403	2	$ 35,730,806
HXT-104	$ 10,682,959	2	$ 21,365,918
HXT-105	$ 2,665,981	2	$ 5,331,962
HXT-106	$ 951,923	2	$ 1,903,847
HXT-107	$ 494,227	2	$ 988,454
HXT-501	$ 989,117	2	$ 1,978,234
HXT-401	$ 156,982	2	$ 313,963
CT-101	$ 865,615	2	$ 1,731,230
CT-102	$ 848,691	1	$ 848,691
CT-103	$ 834,566	1	$ 834,566
P-101	$ 284,719	2	$ 569,439
P-401	$ 67,093	2	$ 134,185
P-201-9 A/B	$ 28,317	18	$ 509,697
P-501	$ 36,579	2	$ 73,157
P-603	$ 15,805	2	$ 31,609
P-604	$ 22,085	2	$ 44,170
P-602	$ 32,092	2	$ 64,184
P-601	$ 15,115	2	$ 30,229
VSS-401	$ 38,584	2	$ 77,168
VSS-402	$ 622,409	2	$ 1,244,818
VSS-501	$ 445,310	2	$ 890,619
F-401	$ 55,860	2	$ 111,721
E-401	$ 260,772	2	$ 521,543
EV-401	$ 55,860	2	$ 111,721
F-601	$ 50,836	2	$ 101,673
F-603	$ 53,479	2	$ 106,958
F-602	$ 167,408	2	$ 334,815
D-601	$ 68,781	2	$ 137,563
HT-603	$ 50,000	2	$ 100,000
HT-601	$ 50,000	2	$ 100,000
HT-501	$ 15,000	2	$ 30,000
HT-301	$ 15,000	2	$ 30,000
HT-602	$ 89,500	2	$ 179,000
SMB-301A/B	$ 4,871,593	1	$ 4,871,593
SMB-201-5A/B	$ 173,985,476	1	$ 173,985,476
Total Estimated Cost			**$285,000,000**

Table #5 Equipment Costs

The largest cost of equipment is the SMBC units at almost $174 million. These are vital pieces of equipment for the plant as without them separation of the reduced sugars would become more time-consuming, and our plant would become less profitable. As SMB technology is still relatively new in industry, pricing of these units at our scale likely has a lot of variability.

Annual costs for the plant are summarized below in Table #6. Wages and Maintenance were calculated using Seider et al. (27) and benefits for workers were calculated based on a percentage of salaries (17). Utilities and wastewater management costs were calculated from Peters et al. The stationary phase cost for SMBC was determined from Xie et al. The remaining chemistry costs were found from online marketplaces which had a lot of variability in prices, so these prices are likely to fluctuate.

Direct Wages	$15,110,000
Benefits	$3,260,000
Chemistry	
34% HCL	$1,000
DMC	$23,470,000
Process Water	$870,000
SMB Stationary Phase	$146,060,000
Catalyst	$4,000
Membrane	$7,000
Waste Management	$112,820,000
Utilities	$20,940,000
Matinance	$47,310,000
Annual Costs	**$369,852,000**

Table #6 Annual Costs

The two largest annual costs are the SMBC stationary phase and wastewater management. The SMBC stationary phase cost was annualized based on its 7-year lifespan. The

wastewater management cost is very high due to the large amount of water that is not recycled in the end process. This cost could be brought down further through the addition of other unit ops, but that was omitted due to the increasing complexity and scale of the current project.

A cash flow analysis was performed and summarized below in table #7.

Year	Depreciable Capital Investment	Working Capital	Depreciation	Annual Cost (excluding Depreciation)	Annual Sales	Net Earn	Cash Flow	Cum PV
1	$ (71,250,000)						$ (71,250,000)	$ (71,250,000)
2	$ (71,250,000)						$ (71,250,000)	$ (130,625,000)
3	$ (142,500,000)	$ (2,000,000)					$ (144,500,000)	$ (230,972,222)
4			$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 439,813,140	$ 23,549,271
5			$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 439,813,140	$ 235,650,515
6			$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 439,813,140	$ 412,401,552
7			$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 439,813,140	$ 559,694,083
8			$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 439,813,140	$ 682,437,858
9			$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 439,813,140	$ 784,724,338
10			$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 439,813,140	$ 869,963,071
11			$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 439,813,140	$ 940,995,348
12			$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 439,813,140	$ 1,000,188,913
13		$ 2,000,000	$ 28,500,000	$ 369,852,000	$ 1,051,230,000	$ 411,313,140	$ 441,813,140	$ 1,049,741,197

Table #7 Cash Flow Analysis

The first 3 years are devoted to building the plant and installing the equipment. Straight line depreciation was assumed for the equipment, based on a 10-year lifespan, and a tax rate of 37% was chosen for calculating the earned value. The IRR for the 13-year timeline was 53%, and the NPV was over $1 billion. This shows that the proposed plant would be very profitable, but there are still some aspects that need further research.

One aspect that needs to be further investigated is the logistics of receiving the agro-waste. Our proposition for this plant currently assumes that the waste is received for free, but the cost of shipping the waste across the state was not calculated. This would likely be a high cost and could greatly impact the plant profitability. The most economical and environmental solution

would likely be to transport the waste via train to the plant location and then the last mile transportation via semi-truck.

Conclusions and Recommendations

This proposed plant in its current state produces over 8,200 metric tons of HMF every year for a total amount of sales of 820 million dollars, and another 224 million dollars is brought in from reduced sugars. The plant uses over 105 million gallons of water per year and has a total energy usage of over 35,000 kW.

While there were many optimizations done to get to this position, the two main ones included adding a water recycle loop and a byproduct purification section. The water recycling loop was necessary and decreased the plant's water usage by over 60%. This was achieved by pulling water from the SMB waste streams which were over 99% pure in water, as well as the steam condensate from the byproduct purification. The byproduct purification was added which involved many different unit ops to purify the various byproducts from SMBC. After purified, they could then be sold to supplement various other plant costs and ended up accounting for around 20% of the total plant income.

Although the plant in its current state has a NPV of over 1 billion dollars and an IRR of 53%, there are still a few factors that could affect whether the plant should be constructed. The first of which is the logistics of getting the agro-waste to the plant. As the transportation of the waste was not accounted for in the cost analysis it would need to be considered as this would likely increase the annual costs and environmental output of the plant. Another factor to consider is the use of SMBC. Due to the complexity of the process many simplifications and assumptions had to be made, and as SMBC is a vital part of the plant further research needs to be completed to use SMBC at this scale. Lastly research into using granular activated carbon should be explored as a purification step after the conversion of fructose to HMF to ensure a 95% purity.

Due to the current high NPV and IRR we believe that this plant should be constructed after the proper research is done.

Nomenclature

HMF: 5-Hydromethylfurfural

DMF: 2,5 – Dimethylfuran

SMB: Simulated Moving Bed

SMBC: Simulated Moving Bed Chromatography

SWH: Subcritical Water Hydrolysis

PFD: Process Flow Diagram

NPV: Net Present Value

IRR: Investor Rate of Return

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Appendices

Table #8: Equipment Summary

Heat Exchangers	***HXT-101***	***HXT-102***	***HXT-103***	***HXT-104***	***HXT-105***	***HXT-106***
Type	Shell and Tube	Shell and Tube	Shell and Tube	Shell and Tube	Shell and Tube	Shell and Tube
Pressure (MPa)	0.1	0.1	30	30	30	0.1
HE Area (ft^2)	16872	1388	24151	14753	2761	6145
Heat duty (kW)	26019	2808	13745	11885	2987	2808
Orientation	Horizontal	Horizontal	Horizontal	Horizontal	Vertical	Vertical
MOC	316 SS	316 SS	316 SS	316 SS	316 SS	316 SS
	HX-107	***HXT-401***	***HXT-501***			
Type	Shell and Tube	Shell and Tube	Shell and Tube			
Pressure (MPa)	0.1	2	0.1			
HE Area (ft^2)	2510	61.4	1.5			
Heat duty (kW)	2809	658	N/A			
Orientation	Vertical	Horizontal	Vertical			
MOC	316 S	Monel Steel	316 SS			
Pumps	***P-101***	***P-201-9 A/B***	***P-601***	***P-602***	***P-603***	***P-604***
Flow rate (gal/min)	369	74	14.4	210	16.9	24.1
Power (hp)	33.0556	7.3	0.9	20.7	1	1.5
MOC	316 SS	316 SS	316 SS	316 SS	316 SS	316 SS
Flash Drums	***F-401***	***F-601***	***F-602***	***F-604***		
Volume (L)	200	936	14045	1050		
Heat Duty (kW)	117.4	1606	24381	3080		

Residence Time (min)	1	17	17	17		
MOC	Monel Steel	316 SS	316 SS	316 SS		
Separators/Splitters	***SP-101***	***SP-102***	***S-101***	***S-301***		
MOC	316 SS	316 SS	316 SS	316 SS		
Valve	***V-101***	***V-401***				
Type	Pressure Relief	Pressure Relief				
Pressure in (MPa)	30	2				
Pressure out (MPa)	1	0.1				
MOC	316 SS	Monel Steel				
Vessels	***HT-301***	***VSS-401***	***VSS-402***	***VSS-501***	***HT-501***	***HT-601***
Volume (L)	20000	500	500	13444	20000	60000
Orientation	Vertical	Vertical	Vertical	Vertical	Vertical	Vertical
MOC	316 SS	316 SS	Monel Steel	316 SS	316 SS	316 SS
	HT-602	***HT-603***				
Volume (L)	250000	60000				
Orientation	Vertical	Vertical				
MOC	316 SS	316 SS				
Simulated Moving Bed	***SMB-201 A/B***	***SMB-202 A/B***	***SMB-203 A/B***	***SMB-204 A/B***	***SMB-205 A/B***	***SMB-301 A/B***
Column Volume (L)	7068	7068	7068	7068	7068	7068
# of Columns	20	20	20	20	20	8
MOC	316 SS	316 SS	316 SS	316 SS	316 SS	316 SS
Evaporator	***EV-401***					

Volume (L)	200		
Temp (C)	40		
Pressure (MPa)	0.1		
Heat Duty (kW)	1151		
Orientation	Vertical		
MOC	Monel Steel		
Extractor	***E-401***		
Volume (L)	200		
Orientation	Vertical		
MOC	Monel Steel		
Distillation Column	***D-601***		
Volume (L)	1860		
Heat Duty (kW)	2202		
Orientation	Vertical		
MOC	316 SS		
Membrane	***MM-501***		
Area (m2)	447		
MOC	PDMS		
Mixers	***M-101***	***M-102***	***M-601***
Orientation	Vertical	Vertical	Vertical
MOC	316 SS	316 SS	316 SS
Cooling Towers	***CT-101***	***CT-102***	***CT-103***
Cooling Tons	1995	1955.5	1922.9
Temp Difference (C)	18.43	18.43	18.43

Orientation	Vertical	Vertical	Vertical
MOC	Cement	Cement	Cement

Table #9: Stream Table for Subcritical Water Hydrolysis

Stream Name	SMB	COOLING	D1	D2	L1	L2	L3	P1	P2	P3	P4	P5
Temperature (°C)	70	25	60	92.47	230	96.33	213.69	25	25	100.02	100.02	80.30
Pressure (bar)	1.01	1.01	1.01	1.01	30	30	30	1.01	1.01	1.01	1.01	1.01
Component Mass Flow (kg/hr unless specified)												
Water	151200	159960	72000	72000	75600	75600	75600	318000	18000	18000	318000	318000
Xylose	0	0	0	0	0	0	0	0	0	0	0	0
Furfural	0	0	0	0	0	0	0	0	0	0	0	0
Arabinose	0	0	0	0	0	0	0	0	0	0	0	0
Pecan Shells	0	0	0	0	0	0	0	0	0	0	0	0
Dextrose/Glucose	0	0	0	0	0	0	0	0	0	0	0	0
Cellobiose	0	0	0	0	0	0	0	0	0	0	0	0
HMF	0	0	0	0	0	0	0	0	0	0	0	0

Table #10: Stream Table for Subcritical Water Hydrolysis

Stream Name	P6	P7	P8	P9	PEC DUST	REC YCLE	RESI DUE	S1	S2	S3	S4	S5
Temperature (°C)	61.87	43.44	25.00	98.26	18.00	100.30	220	78.28	100.02	89.42	91.34	220
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01	300	1.01	1.01	1.01	300	300
Component Mass Flow (kg/hr unless specified)												
Water	318000	318000	300000	300000	0	41459	0	39923	41459	81382	81382	81382
Xylose	0	0	0	0	0	0	0	0	0	0	0	0
Furfural	0	0	0	0	0	0	0	0	0	0	0	0
Arabinose	0	0	0	0	0	0	0	0	0	0	0	0
Pecan Shells	0	0	0	0	20345	0	2747	0	0	0	0	0
Dextrose/Glucose	0	0	0	0	0	0	0	0	0	0	0	0
Cellobiose	0	0	0	0	0	0	0	0	0	0	0	0
HMF	0	0	0	0	0	0	0	0	0	0	0	0
Water	318000	318000	300000	300000	0	41459	0	39923	41459	81382	81382	81382

Stream Name	S6	S7	S8	S9	S10	GLUC TO FRUC	SMB UTILI TY	TO SMB	WATE RIN
Temperature (°C)	220	220	117	90	95.43	70	70	70	18
Pressure (bar)	300	300	300.00	300	1.01	1.01	1.01	1.01	1.01
Water	81382	81382	81382	81382	81382	8760	159960	81382	39923
Xylose	12146	12146	12146	12146	12146	0	0	12146	0
Furfural	2645	2645	2645	2645	2645	0	0	2645	0
Arabinose	1139	1139	1139	1139	1139	0	0	1139	0
Pecan Shells	2747	0	0	0	0	0	0	0	0
Dextrose/Glucose	671	671	671	671	671	0	0	671	0
Cellobiose	224	224	224	224	224	0	0	224	0
HMF	773	773	773	773	773	0	0	773	0
Water	81382	81382	81382	81382	81382	8760	159960	81382	39923

Table #11: Stream Table for Simulated Moving Bed

Stream Name	D1	D2	D3	D4	D5	D6	F1	F2	F3	F4	F5	F6
Temperature (°C)	75	75	75	75	75	75	75	75	75	75	75	75
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01
Component Mass Flow (kg/hr unless specified)												
Arabinose	0	0	0	0	0	0	127	126	125	0	0	0
Glucose	0	0	0	0	0	0	75	74	74	73	73	0
HMF	0	0	0	0	0	0	86	85	0	0	0	0
Furfural	0	0	0	0	0	0	294	0	0	0	0	0
Xylose	0	0	0	0	0	0	1350	1343	1336	1329	0	0
Cellobiose	0	0	0	0	0	0	25	25	25	24	24	24
Water	3000	3000	3000	4800	3000	16800	9042	9042	9042	9042	9042	9042

Stream Name	W1	W2	W3	W4	W5	Glucose	Fur fural	Ara binose	HMF	Xylose
Temperature (°C)	75	75	75	75	75	75	75	75	75	75
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01
Arabinose	0.63	0.63	0.63	0	0	0	0	124.70	0	0
Glucose	0.37	0.37	0.37	0.37	0.37	72.75	0	0	0	0
HMF	0.43	0.43	0	0	0	0	0	0	85.05	0
Furfural	1.47	0	0	0	0	0	292.41	0	0	0
Xylose	6.75	6.71	6.68	6.65	0	0	0	0	0	1322.79
Cellobiose	0.12	0.12	0.12	0.12	0.12	0	0	0	0	0
Water	1830.36	2659.82	2501.2	831.63	2708.99	291.01	1169.64	498.82	340.18	3968.37

Table #12: Stream Table for Byproduct Purification

Stream Name	FEED ARA	FEED DEX	FEED HMF	FEED XYL	PARA	PDEX	PHMF	PXYL	REC YCLE	WAT ER1	WAT ER3	WATE R4	WATE R5
Temperature (°C)	70	75	75	75	135	107	122	135	100	107	135	100	135
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01
Component Mass Flow (kg/hr unless specified)													
Glucose	0	655	0	0	0	655	0	0	1.27 E-04	1.27 E-04	0	0	0
HMF	0	0	765	0	0	0	765	0	2.01 E-11	0	0	2.01 E-11	0
Arabinose	2808	0	0	0	2802	0	0	0	5.89	0	0	0	5.89
Furfural	0	0	0	0	0	0	0	0	0	0	0	0	0
Xylose	0	0	0	11905	0	0	0	11747	158	0	158	0	0
Cellobiose	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	1348	2619	3062	35715	168	237	38	842	41459	2382	34873	3024	1179

Table #13: Stream Table for Furfural Recovery

Stream Name	C1	C2	F1	F2	F3	F4	P1	R1
Temperature (°C)	64.85	64.85	64.85	64.85	64.85	64.85	64.85	64.85
Pressure (bar)	0.003	0.003	0.003	0.003	0.003	0.003	0.003	0.003
Component Mass Flow (kg/hr unless specified)								
Furfural	0	0	2688	2688	2688	2688	2661	27
Water	10526	10526	0	0	10526	10526	142	10384

Table #14: Stream Table for Glucose to Fructose Conversion

Stream Name	F1	F2	F3	D1	P1	W1	G1
Temperature (°C)	25	45	25	25	25	25	25
Pressure (bar)	1	1	1	1	1	1	1
Component Mass Flow (kg/hr unless specified)							
GLUCOSE	655	301	300	0	0	0	300
WATER	0	2619	5780	2619	0	5780	0
FRUCTOSE	0	354	1.06	0	354	0	1.06

Table #15: Stream Table for Fructose to HMF

Stream Name	AQ	COLD IN	COLD OUT	DMC	DMC ADD	DMC REC	EX HMF	FRU	HCL	HMF	ORG	TOEX
Temperature (°C)	191	25	92	25	25	101	100	25	25	101	41	40
Pressure (bar)	1	1	1	1	1	1	1	1	1	1	1	1
Component Mass Flow (kg/hr unless specified)												
Fructose	7	0	0	0	0	4.14 E-02	6.64	354	0	5.67	5.71	12.38
DMC	3604	0	0	3759	1.00E-03	1581	238	0	0	156	1737	3759
Water	1210	8293	8293	0	0	522	106	0	2.27 E-02	69	591	1279
HCl	7.22E-03	0	0	0	0	9.09 E-06	3.54 E-06	0	1.34 E-02	0	6.17 E-03	1.34 E-02
HMF	129	0	0	0	0	4.72 E-01	128	0	0	110	110	239

Stream Name	TOHXT	TOPUMP	TORCT	TOSWH	TOV	TOV2	WATER
Temperature (°C)	200	25	28	100	40	25	25
Pressure (bar)	20	1	20	1	20	1	1
Component Mass Flow (kg/hr unless specified)							
Fructose	12	354	354	6.64E-02	12.38	354	0
DMC	3759	3759	3759	3365	3759	0	0
Water	1279	1176	1176	1104	1279	1176	1176
HCl	1.34 E-02	1.34E-02	1.34E-02	7.21E-03	1.34 E-02	0	0
HMF	239	0	0	7.40E-01	239	0	0