Production Plant of Nanoparticle Mineral Oxide Sunscreen

A Technical Report submitted to the Department of Chemical Engineering

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On my honor as a University Student, I have neither given nor received unauthorized aid on this assignment as defined by the Honor Guidelines for Thesis-Related Assignments

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1. Summary

This technical report covers the proposed design of a production plant within the United States to manufacture a broad-spectrum sunscreen made with zinc oxide and titanium dioxide nanoparticles. Through our design and formulation, we plan to bring accessibility to the sunscreen market by designing a more affordable product than competitors, more effective at protecting against damaging ultraviolet rays, and a product rich with skincare ingredients.

The production plant includes three main processes: zinc oxide nanoparticle synthesis, titanium dioxide nanoparticle synthesis, and the emulsification of the sunscreen product. The plant is designed to produce 5.2 million fl oz per year, making 5.2 million units of 1 fl oz bottles of sunscreen. Each sunscreen will be sold for $10.00 wholesale. Packaging will be handled at a different facility.

The production plant will be located in Austin, Texas. The two revenue streams come from selling the sunscreen for-profit and isopropyl alcohol from our titanium dioxide synthesis process. After startup, the expected revenue from the plant will be $52,507,000 per year. Additionally, our plant is expected to break even within the first year of production. The after-tax ROI increases annually by 446%.

2. Introduction

The U.S. Food and Drug Administration (FDA) began to regulate sunscreen in 1978 after classifying sunscreen as an over-the-counter drug (Aldahan et al., 2015). As a result, ingredients found in sunscreens are subject to approval by the FDA. The process is time-consuming and strict, and as a result, only 16 ingredients are approved (21 CFR 352.10). No new ingredients have been approved since 1999. Two ingredients on the list are zinc oxide (ZnO) and titanium dioxide (TiO_2), which have been regulated since the 1990s and are generally recognized as safe (FDA, 2021). The metal oxides also typically sit on top of the skin and do not penetrate it, preventing irritation (Gamer et al., 2006). They have also been found to be non-comedogenic, or non-pore-clogging. This makes the ingredients more desirable, especially for acne-prone or sensitive skin. All these factors make the metal oxides popular active ingredients in sunscreens.

While these ingredients make sunscreens effective, a lot of these sunscreens can leave an undesired white cast. This is more prominent in people with darker complexions. This is due to these metal oxides being naturally white. However, synthesizing mineral oxides as nanoparticles works around the white cast problem. The human eye generally sees particles as small as 40-50 microns (Close, 2023). So, by making the metal oxides nanoparticle-sized, they are invisible to the human eye without any aid. Nanoparticles are still as effective as their larger counterparts at filtering UV light (Otanicar et al., 2016). Therefore, the white cast that would be left on the skin would be eliminated without any additives, such as pigmentation for tinting.

This project will focus on developing sunscreen using nanoparticle-sized metal oxides to ensure protection against UV rays and eliminate the white cast associated with mineral sunscreen usage.

3. Previous Work

An important resource for this project was a previous capstone project on sunscreens from UVA Chemical Engineering students. This project was published in 2017 by Raleigh Heap, Marguerite Osmundsen, Carly Markbreiter, and Shivanni Sukha. Their project synthesizes ZnO nanoparticles and vitamin E to create their sunscreens. However, we wished to improve their project by increasing the scale and modifying certain process steps. Modifications and improvements included:

a. Scale-up in production. The previous capstone produced 240,000 fl oz in a year, while our project aimed to produce 5.2 million fl oz per year. The difference in amounts is due to an increase in the market for sunscreens in the last few years.

b. Direct-precipitation method instead of sol-gel. The sol-gel method allows for more precise control over the composition and size of nanoparticles. However, these require a more controlled environment. Direct precipitation may lead to a less uniform distribution of nanoparticle sizes but allow for a larger amount to be synthesized simultaneously. This is addressed by adding extra operating units that will bring the nanoparticles to the target size.

c. Addition of TiO_2 nanoparticles as an active ingredient. The previous capstone only used ZnO as its active ingredient. While ZnO is already effective alone, TiO_2 provides additional protection against UVB rays.

d. Improved formulation. The previous capstone had vitamin E antioxidants and polymerized soybean oil to address the texture and appearance of their sunscreen. Our final formulation composition is based on a paper that provides the composition of a typical sunscreen (Pawlowski & Petersen-Thiery, 2020). This ensures that sunscreen would match the texture and consistency of other sunscreens on the market.

4. Discussion

4.1. Process Scale

In 2023, the global sun care market was valued at approximately USD 14.35 billion, with an expected annual growth rate of 6.1% (Grand View Research, 2022). This puts the estimated 2024 market size at around USD 15.23 billion. Within this market, the lotions/creams segment accounts for 42.7%, approximately USD 6.5 billion. This segment includes various adult cream-based sunscreens: chemical, traditional mineral, and nanoscale mineral types.

To refine our target market, we examine companies with similar products to our proposed sunscreen. The Honest Company, a producer of personal and skin care products, reported USD 88.104 million in revenue from skin and personal care in 2023 (The Honest Company, 2024). Assuming all this revenue came from sunscreen sales, this represents about 1.36% of the total lotions/creams sun care market in the U.S. This market share aligns well with the anticipated scale of our production.

Using the Honest Company's revenue as a reference, we can estimate potential sales volume. With their mineral sunscreen at a retail price of USD 17 per fluid ounce, we calculate they sold approximately 5,200,000 fl oz or about 198,000 kg of sunscreen annually. This provides a useful benchmark for our production volume, assuming a similar market scope.

For our sunscreen, an SPF 30 formulation requires ZnO and TiO_2 concentrations (w/w) of 15-20% and at least 5%, respectively. Thus, our sunscreen will contain 15% ZnO and 5% TiO_2 with the remainder comprising preservatives, stabilizers, and other purchased ingredients. Annually, this translates to production requirements of 29,742 kg of ZnO and 9,914 kg of TiO_2 to produce 5,200,000 fl oz of sunscreen per year. Using a traditional composition of mineral sunscreen products, the weight percentage of purchased ingredients includes 5% caprylic triglyceride, 5% glycerin, 5% glyceryl stearate, 1% styrene/acrylate copolymer, 2% tridecyl salicylate, 2% dimethicone, and 60% water which are added proportionally during our process (Pawlowski & Petersen-Thiery, 2020).

4.2. Zinc Oxide Nanoparticle Synthesis

ZnO is a mineral that can reflect UVB and UVA radiation, protecting the skin from damaging ultraviolet radiation that can lead to skin damage and skin cancer. ZnO is synthesized by combining zinc nitrate and sodium hydroxide (NaOH) in a direct precipitation reaction to form a precipitate of ZnO nanoparticles in a batch reactor. This is then centrifuged and washed repeatedly with water to remove the remaining starting product and other byproducts. A wet cake of water and nanoparticles is left from these processes. The wet cake is sent to a rotary dryer to be completely dried. The now-dried powder is then sent to a miller to grind the nanoparticles to the correct particle size. The process flow diagram (PFD) is found in Figure 5.2.2.

4.2.1. Mixing Design & Scale-Up

Before the reaction to produce ZnO can proceed, the zinc nitrate hexahydrate needs to be prepared in a solution. Zinc nitrate hexahydrate (ZNH) is sourced as a solid and must be dissolved in water. Water is first loaded into a mixing tank (MT-1) and then the ZNH is charged. MT-1 is stirred to ensure complete dissolution. Material balances were used to determine the appropriate amount of water and ZNH such that the proper molarity was achieved. The volume of MT-1 was determined based on 80% of its capacity being designated as the working volume. Furthermore, the impeller diameter was found using Equation 4.2.1-1.

$$3D_a \approx D_T \tag{4.2.1-1}$$

Mixing parameters were determined by using a heuristic of a 5 m/s tip speed. Based on various mixing techniques, average tip speeds are 3-6 m/s, so 5 m/s was chosen. From there, rotations per minute (RPMs) were found. We verified that mixing at this speed gave results in the turbulent regime using Reynolds number calculations. Using the density of the solution and the parameters previously mentioned, the power was found for mixing, given the use of a pitched blade impeller.

Calculations are found in Appendix A.2.1. MT-1 is an INDCO SST-800 mixing tank with a volume of 800 gallons and mixed at 190 RPM. The impeller diameter is 0.5 m. The power requirement is 12.1 kW, and the liquid will be mixed for 20 minutes to ensure complete dissolution.

The direct precipitation of ZnO starts by mixing a solution of NaOH and zinc nitrate in water, such that the concentrations are 0.5 M of Zn^{2+} and 1.0 M of OH^-. The reaction yield is 90% (Wu et al., 2006), which is accounted for in the material balances. The NaOH solution is charged into the stirred reactor (SR-1) first, and then the zinc nitrate solution is added overhead using a showerhead discharge. The mixture is stirred at 90°C. The parameters for the stirred reactor were scaled up from literature findings (Wu et al., 2006). To determine mixing time, the equation found below equates relative impeller diameter sizes to mixing time (Geankoplis, 1993). In this equation, t_{t2} represents the time the reaction takes at large scale, while t_{t1} represents the time it took based on lab-scale from literature. D_{a2} and D_{a1} represent diameter at large scale and lab scale respectively.

$$\frac{t_{t2}}{t_{t1}} = \left(\frac{D_{a2}}{D_{a1}}\right)^{\frac{11}{18}} \qquad (4.2.1\text{-}2)$$

The volume of SR-1 and the impeller diameter were found based on the same principles described for MT-1. The power and mixing speed were found retroactively by using a power-to-volume ratio based on the values in a previous capstone report (Suhka, 2017). Keeping the power number constant, and using a pitched blade impeller, the Reynolds number was confirmed to remain in the turbulent regime. The equations listed below were used to identify these parameters.

$$N_p = \frac{P}{n^3 {D_a}^5 \rho} \qquad (4.2.1\text{-}3)$$

$$Re = \frac{{D_a}^2 n \rho}{\mu} \qquad (4.2.1\text{-}4)$$

Relevant calculations and results are found in Appendix A.2.2. SR-1 is a Pfaudler mixing tank with a volume of 1000 gallons. The reaction will occur in SR-1 over 13.2 hours.

For the first 2.6 hours (⅕ of the mixing time based on the study conducted by Wu et al.) in SR-1, the zinc nitrate solution will be added gradually overhead. The impeller diameter is 0.61 m and the diameter of SR-1 is 1.83 m. The power needed to mix the reagents in the report by Suhka was 869 W and the volume of the tank was 50 L. This is approximately 50 times smaller than our scale, thus a scaled power of 42 kW was determined. From there, the mixing speed was found using McCabe Figure 9.13 (Appendix A.2.2) to be 226 RPM. The precipitate and solution from SR-1 will be pumped into a centrifuge to isolate the solid mass for further processing. Refer to section 4.6.1 and Appendix A.10 for energy balance calculations regarding the reaction occurring in SR-1.

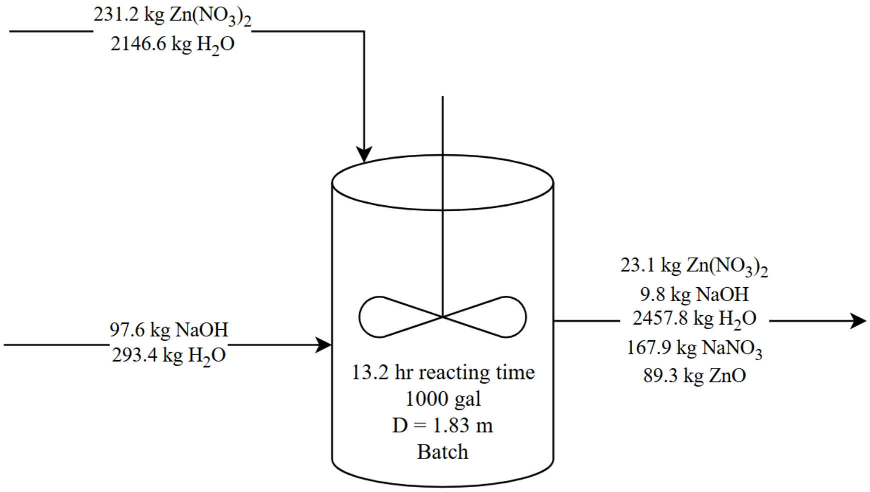

Figure 4.2.1: Mass balance schematic for ZnO synthesis reactor, SR-1

4.2.2. Centrifugation and Washing

Once the ZnO nanoparticles have been synthesized, multiple rounds of washing are required to remove residual precursor materials and byproducts. The disk stack centrifuge was selected for its ability to effectively separate fine nanoparticles from the liquid phase in two-phase systems. This centrifuge operates by rotating the suspension within a bowl containing multiple stacked disks that divide the flow into thin layers, enhancing separation efficiency. The centrifugal force drives the denser ZnO nanoparticles outward, where they accumulate along the bowl’s periphery, while the liquid phase is expelled.

The selection of the disk stack centrifuge was based on the material volume, particle characteristics, and liquid phase composition. The ZnO nanoparticles exit the reactor at an average size of 200 nm and are suspended in the reactor effluent. The settling velocity, which establishes the speed at which a particle settles out of a fluid, and the separation time, which accounts for the amount of time it takes for the particle to settle out of the fluid, are determined from these equations:

$$V_t = \frac{g {d_p}^2(\rho_p - \rho_s)}{18\mu_s} \qquad (4.2.2\text{-}1)$$

$$t = \frac{x}{V_t} \qquad (4.2.2\text{-}2)$$

At an operating G-force of 12,000×g, the settling velocity of the nanoparticles was calculated as 0.52 mm/s. Given a typical separation distance of 5 cm, the estimated separation time is approximately 42 seconds. With a batch volume of 2640 L, the centrifuge needs to be able to process the nanoparticles completely as well as in a timely manner. The Flottweg AC1000 Separator was selected to meet these operational demands. A photo is shown in Figure 4.2.2 and a cross-sectional view in Figure 4.2.3. The Flottweg AC1000 Separator is capable of processing up to 10,000 L/h and achieving a maximum G-force of 12,000×g, making it well-suited for this application. With a total solution volume of 2640 L, the necessary centrifugation time is approximately 16 minutes, which is sufficient for complete separation of the nanoparticles. All relevant calculations are found in Appendix A.2.3.

Figure 4.2.2: Flottweg AC 1000 Separator (https://www.flottweg.com/fileadmin/user_upload/data/pdf-downloads/Separator-EN.pdf)

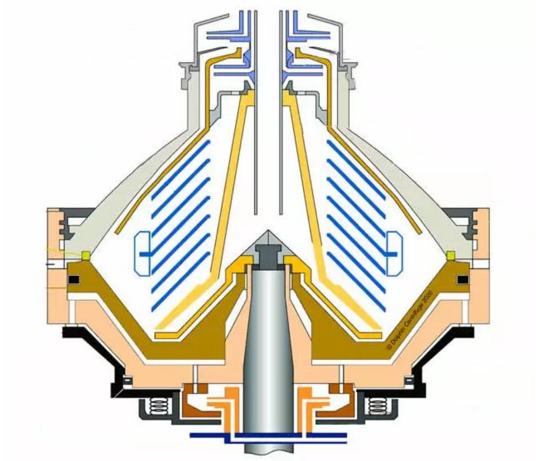

Figure 4.2.3 Cross-Section of Disk Stack Centrifuge (https://dolphincentrifuge.com/disc-centrifuge-parts-glossary/)

Following the centrifugation step, the ZnO is collected as a wet cake with an assumed water content of 50% by volume. This wet cake is then transferred to a mixing tank, MT-2, and resuspended in water at a solid-to-liquid ratio of 1:154. The volume, dimensions, and impeller diameter were determined from the methods described for MT-1, and the mixing speed was found by assuming a tip speed of 5 m/s. The Reynolds number was found using the density of the solution with the suspended precipitate. Power was found using power number correlations for high-shear Rushton impellers. A high-shear impeller is necessary for this suspension to occur and break up large masses. Ample mixing time was given for each wash cycle in MT-2.

Calculations are found in Appendix A.2.4. MT-2 is a 1000-gallon (3786 L) Pfaudler tank with an impeller diameter of 0.61 m. The mixing speed needs to be 156 RPMs. The power required for an impeller of this size and speed is 7.6 kW. Each wash cycle will take 15 minutes. The resuspended mixture undergoes two additional centrifugation cycles, each followed by resuspension in fresh water to ensure the complete removal of impurities, byproducts, and unreacted precursor materials. After the third centrifugation cycle, which totals approximately 2 hours of washing and centrifugation, the ZnO wet cake is transferred to a dryer for further moisture removal. The stream breakdown and each resuspension step of this process is found below in Table 4.2.2.

Table 4.2.2 Stream Table for ZnO Washing and Centrifuging

Stream Name	Z5	Z6 - After all washes	Z7	Z8	Z9	Z10
kg/batch	2747.9	7526.5	105.2	2410.1	2515.3	105.2
From	SR-1	C-1	C-1	Water Feed	MT-2	C-1
To	C-1	Waste	MT-2	MT-2	C-1	D-1
Component Breakdown (kg/batch)						
ZnO	89.3	0	89.3	-	89.3	89.3
ZNH	-	-	-	-	-	-
$Zn(NO_3)_2$	23.1	23.1	-	-	-	-
NaOH	9.8	9.8	-	-	-	-
$NaNO_3$	167.9	167.9	-	-	-	-
H_2O	2457.8	7325.7	15.9	2410.1	2426	15.9
Air	-	-	-	-	-	-

Table 4.2.2 (cont.) Stream Table for ZnO washing and Centrifugation

	Resuspension 1				Resuspension 2				Resuspension 3			
Stream Name	Z6	Z7	Z8	Z9	Z6	Z7	Z8	Z9	Z6	Z7	Z8	Z9
kg/batch	2642.7	105.2	2441.9	2457.8	2441.9	105.2	2441.9	2547.1	2441.9	105.2	2441.9	2547.1
From	C-1	C-1	Water Feed	MT-2	C-1	C-1	Water Feed	MT-2	C-1	C-1	Water Feed	MT-2
To	Waste	MT-2	MT-2	C-1	Waste	MT-2	MT-2	C-1	Waste	MT-2	MT-2	C-1
Component Breakdown (kg/batch)												
ZnO	0	89.3	-	89.3	0	89.3	-	89.3	0	89.3	-	89.3
ZNH	-	-	-	-	-	-	-	-	-	-	-	-
$Zn(NO_3)_2$	23.0	0.1	-	0.1	0.1	0	-	0	0	0	-	0
NaOH	9.7	0.1	-	0.1	0.1	0	-	0	0	0	-	0
$NaNO_3$	166.9	1.0	-	1.0	1.0	0	-	0	0	0	-	0
H_2O	2443.1	14.7	2441.9	2456.6	2440.7	15.9	2441.9	2457.8	2441.9	15.9	2441.9	2457.8
Air	-	-	-	-	-	-	-	-	-	-	-	-

4.2.3. *Drying, Milling, & Sizing*

The ZnO nanoparticles are dried using a direct counter-current dryer. The oxide is not heat-sensitive, and counter-current flow allows for better thermal efficiency. The nanoparticle wet cake is exposed to a controlled stream of heated air to remove water. All the wet cake from the previous step is added at once, and the drying process takes approximately an hour to completely dry. The evaporated water will be released into the atmosphere. Dimensions of the rotary dryer were selected using a table from FEECO's typical rotary data table to ensure that a dryer could be easily purchased and priced (FEECO International, n.d.). Since the amount processed per batch is small, drums with smaller diameters were selected. The table used can be found in Appendix A.5.1.

The air velocity and cross-section were used to find the volumetric flow rate of air passing through the drum. The air velocity was selected based on an article that lists the airspeed for the drying of grains as 0.25-2.5 m/s (Mesa et al., 2020). A low air velocity was chosen to prevent nanoparticles from being lifted by hot air. We were unable to find articles detailing the drying of nanoparticles in a rotary dryer, however, further research would aid in designing a fully optimized dryer. The mass flow rate is found using the volumetric flow rate and the density of air at the inlet temperature. The density was found using the ideal gas law. The outlet temperature of the air was found by conducting a heat balance. First is the heat required to raise the wet solids inlet to the desired outlet temperature as seen in Equation 4.2.3-1.

$$Q_1 = \dot{m}_{dry,in} * c_{p,dry} * \left(T_{S,2} - T_{S,1}\right) + \dot{m}_{liq,in} * c_{p,liq} * \left(T_{S,2} - T_{S,1}\right) \tag{4.2.3-1}$$

The subscript “dry” refers to the solids component and “liq” refers to the liquid component. The temperatures are assigned to the streams as shown in Figure 4.2.4.

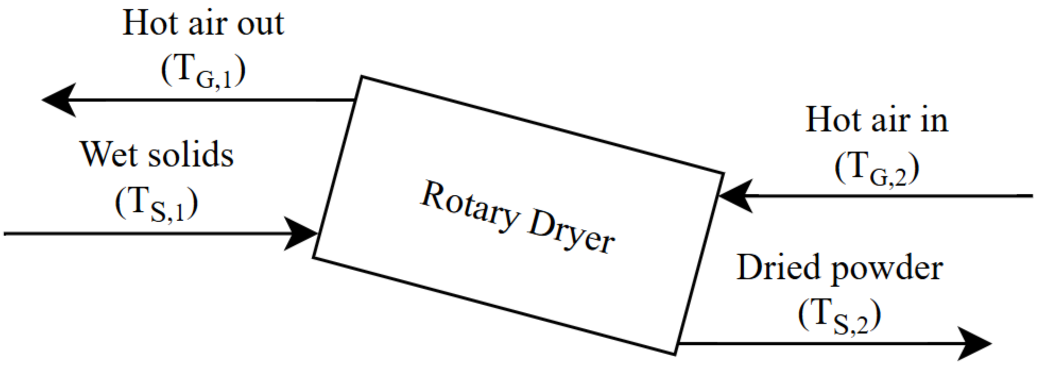

Figure 4.2.4: Diagram of rotary dryer streams and temperatures

Then the heat required to evaporate all the water was calculated using the heat of vaporization using Equation 4.2.3-2 where ΔH_V is at $T_{S,2}$.

$$Q_2 = \dot{m}_{liq,removed} * \Delta H_v(T_{S,2}) \qquad (4.2.3\text{-}2)$$

The total heat required is found by summing the previous heat values. The total heat required can be used to find the outlet temperature of the hot air stream using Equation 4.2.3-3.

$$Q_{tot} = \dot{m}_{air} * C_s * \left(T_{G,2} - T_{G,1}\right) \qquad (4.2.3\text{-}3)$$

The specific heat, C_s, of the system depends on the humidity of the air. The manufacturing plant is located in Austin, Texas. The relative humidity throughout the year is an average of 62% (Weather-And-Climate.com, n.d.). However, for calculations, the highest of the year is used to ensure proper drying throughout the entire year, 71%, at 20°C.

To ensure that no water vapor would condense, the vapor pressure of the outlet air stream was compared to the saturation pressure at the wet cake inlet conditions. The vapor pressure in the air stream was found using Dalton's Law of Partial Pressure and is found in Equation 4.2.3-4.

$$P_i = x_i P_{tot} \qquad (4.2.3\text{-}4)$$

Saturation pressure was found using Antoine's equation. The Antoine parameters were from NIST at the wet solids inlet temperature. It is found in Equations 4.2.3-5.

$$log\ (P_{sat}) = A - \frac{B}{T+C} \qquad (4.2.3\text{-}5)$$

To ensure proper drying, the residence time of the dryer will be one hour. Since the dimensions of the drum are already known, the slope affects the residence time. The residence time is found using Equation 4.2.3-6.

$$\tau = \frac{0.19L}{N*D_{dryer}*tan\ (\theta)} \qquad (4.2.3\text{-}6)$$

To make the drying more efficient, flights are used. Flights move the material inside the drum by lifting, carrying, and dropping it. To calculate the number of flights found inside the drum, a heuristic that it should be equal to three times the diameter in feet was used. The radial height of the flight was found using a heuristic that it should be 1/8th the diameter of the dryer.

All calculations can be found in Appendix A.5.2. The final design of the drum is 1.8 m diameter, 15 m length, 18 flights of 0.23 m radial height, and a slope of 0.76°. The heat required is 41422 kJ/hr and the airflow is 2468 kg/hr. The inlet air temperature is 130°C and the outlet temperature is 114°C. The wet solids enter at 20°C and a dried powder exits at 70°C.

After the drying process, the product consists of approximately 89 kg of ZnO powder with a particle diameter of roughly 200 nm (Wu et al., 2006). However, the desired diameter is around 50 nm, which requires a size reduction. According to research, ZnO nanoparticles in powder form can be dry-milled to achieve the necessary particle size. In this process, high-energy ball milling is used, where a grinding medium breaks apart the particles to reduce their size. Following an established procedure, a 5:1 ratio of grinding medium, in this case, 5 mm hardened steel balls, to ZnO powder is used in the mill per batch (Storion et al., 2021). To decrease the particle size from 200 nm to 50 nm, a milling time of five hours is required.

For this process, the Sweco Vibro-Energy Finishing Mill will be utilized. A photo is shown in Figure 4.2.5. This mill has sufficient capacity to hold the necessary volume for each batch, consisting of 89 kg of ZnO powder and 450 kg of steel balls. Once the milling process is complete, the ZnO powder is reduced to an average particle diameter of 50 nm. According to Storion et al., this process results in a narrow particle size distribution, which ensures that the presence of nanoparticles smaller than 30 nm in diameter is negligible. At this stage, the material is in the proper form for the next steps in sunscreen production and can be stored before being mixed with other ingredients. After milling, the ZnO is stored in a 10-gallon drum. It is later to be discharged for homogenous mixing with TiO_2 in a double cone blender at a bag dump station with a screw feeder.

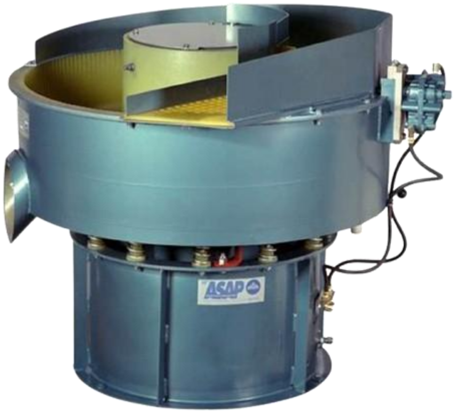

Figure 4.2.5: Sweco Vibro-Energy Finishing Mill
(https://sweco.com/separation/finishing-mill.php)

4.3. Titanium Dioxide Nanoparticle Synthesis

Titanium(IV) isopropoxide (TTIP) at 97% purity is to be combined with alkaline distilled water to create solid TiO_2 and isopropyl alcohol (IPA). The reaction can be seen below:

$$Ti(OCH(CH_3)_2)_4 + 2H_2O \rightarrow TiO_2 + 4(CH_3)_2CHOH$$

The aqueous solution is prepared under temperature-controlled conditions with a cooling jacket, where the alkoxide is added slowly to a stirred reactor, SR-2 (Viana et al., 2010). The precipitate will be filtered and washed repeatedly with deionized water to eradicate any aqueous impurities. The TiO_2 is then dried in a rotary dryer and calcined to ensure the correct nanoparticle size. The IPA generated in the reaction and the water used for the washing steps are collected and sent to distillation. The IPA is recovered and is sold as 70% rubbing alcohol. The PFD for this block of the process is found in Figure 5.2.3.

4.3.1. *Mixing Design & Scale-Up*

The synthesis of TiO_2 nanoparticles begins with the controlled addition of TTIP to deionized water to form a TiO_2 precipitate. This is done in a continuous stirred-tank reactor (CSTR), SR-2, where TTIP and water are added in a mass ratio of 2:3, ensuring an excess of water to promote complete hydrolysis and particle suspension. The reaction occurs at 65°C to facilitate nanoparticle formation. Energy balances relevant to heat transfer for TiO_2 reaction occurring in SR-2 are found in section 4.6.2.

Parameters for the reactor and feed streams were found by determining the output and residence time required for the reaction to occur and keeping pace with the ZnO nanoparticle synthesis process. Reactor sizing was based on the volume of reagents present at any time in the reactor. Then, using the aspect ratio (height of reactor divided by diameter) of 1.5:1, reactor height and diameter were determined, and other sizing metrics (i.e., impeller & baffle width) followed from this ratio. All sizing methods follow a similar approach to tank sizing for ZnO synthesis. These values are expanded upon in Appendix A.4.1. A mass balance around SR-2 can be found in Figure 4.3.1.

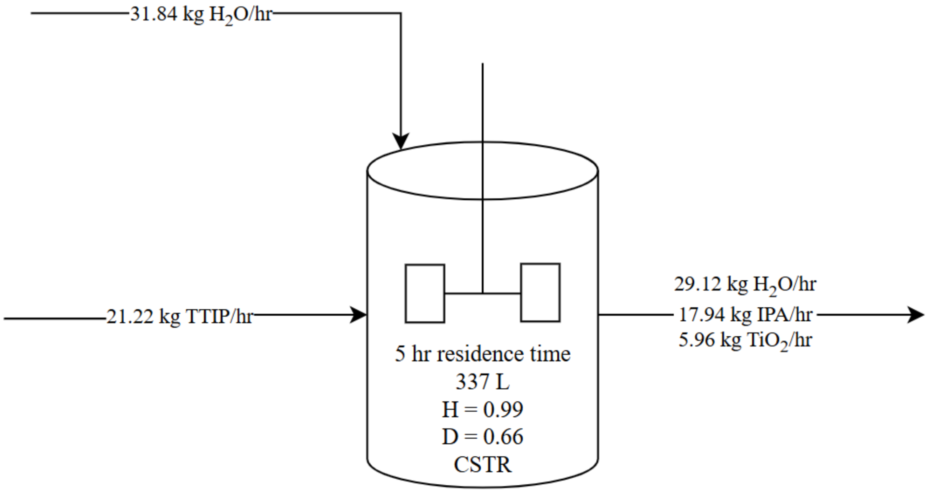

Figure 4.3.1: Mass balance schematic of SR-2 (TiO_2 reactor)

To achieve thorough mixing, a Rushton impeller was selected due to its high shear efficiency and ability to maintain uniform nanoparticle distribution. In previous laboratory studies, mixing times varied from 0.5-10 hours, the most common being 1-2 hours (Buraso, 2018). Extending the residence time beyond this range promotes a higher conversion and growth of our nanoparticle networks. For this reason, a residence time of 5 hours was decided, which produces nanoparticles with an average diameter of 15 nm. This size is too small for our target size (50 nm), so additional downstream processing is implemented to promote further particle growth.

Our final design is a CSTR (337 liters for total volume) with a 5-hour residence time. The tank diameter is 0.66 m, and the impeller diameter is 0.22 m. The power needed to mix the reagents is 93 W at 200 RPM. These values were determined using power-to-volume scaling and Reynolds number calculations, ensuring operation in the turbulent regime.

A CSTR was chosen over ZnO's batch reactor because the reaction happens very quickly ($k = 1.23E14*\exp(-11323/T)\ \mathrm{mol^{-1}cm^{3}s^{-1}}$) and TiO_2 demand (30 kg) is roughly a third of ZnO's (89 kg) (Wei, 2020). The TiO_2 reaction is very quick but produces very small nanoparticles. Our reaction has a 5-hour residence time to encourage nanoparticle diameter growth as there is a relationship between reaction time and particle size (Bade, 2019). Additionally, SR-2's small size and lower operating cost offset the higher initial capital cost. After the reaction proceeds through SR-2, the reactor effluent must be stored for a period to translate the remainder of the processes to batch. Although the reactor SR-2 is run as a CSTR, after the material is collected in MT-3, we will combine 5-hours of flow into a batch. The subsequent washing, drying, and calcining steps are all run as batch processes. Once all the reactor effluent is in the MT-3, additional water is added to get the concentration of particulate optimal for centrifugation. Then, the mixer is powered on to resuspend the precipitate before pumping the effluent to the centrifuge C-2.

The MT-3 dimensions were determined using the same assumptions and calculations as the suspension tank from the ZnO synthesis. These calculations can be found in Appendix A.4.2. MT-3 is an INDCO SST-300 tank with a volume of 300 gallons. The impeller diameter is 0.38 m. The mixing speed must be 250 RPM. Using a high-shear Rushton impeller to ensure suspension and turbulent mixing, the required power is 2.8 kW. The suspension will be mixed for 20 minutes, and then the contents of MT-3 will be pumped to centrifuge C-2 to separate the particles from the bulk liquid.

4.3.2. Centrifugation and Washing

Like ZnO synthesis, after direct precipitation and centrifugation, the centrifuge cake needs to be washed and resuspended to rinse away unwanted materials. The Flottweg AC1000 Separator will be used for this operation, allowing for sufficient separation. At a flow rate of 246 L/h, the required separation time is around 2.9 hours. The separation time for TiO_2 is significantly longer than ZnO because TiO_2 (15 nm) is smaller in size than ZnO (200 nm). The resuspension consists of TiO_2 in 50 vol% IPA and 50 vol% water at a solid-to-liquid volume ratio of 1:100, and the following washes are 100 vol% water to wash out our residual IPA. The mass balance breakdown of each wash cycle is found in Table 4.3.2-1.

Table 4.3.2-1 Stream Table for TiO_2 Washing

	Resuspension 1					Resuspension 2				Resuspension 3			
Stream Name	T6	T7	T8	I7	T9	T6	T7	T8	T9	T6	T7	T8	T9
From	C-2	C-2	Water Feed	ST-5	MT-4	C-2	C-2	Water Feed	MT-4	C-2	C-2	Water Feed	MT-4
To	ST-4	MT-4	MT-4	MT-4	C-2	ST-4	MT-4	MT-4	C-2	ST-4	MT-4	MT-4	C-2
kg/batch	794.6	37.0	320.0	354.7	711.7	674.6	37.1	707.9	717.7	707.9	37.1	707.9	717.7
Component Breakdown (kg/batch)													
H2O	705.5	6.6	320.0	80.7	407.3	403.4	3.9	707.9	711.8	704.5	7.3	707.9	717.7
IPA	89.1	0.6	-	274.0	274.6	271.2	3.4	-	3.4	3.4	0.0	-	0.0
TiO2	-	29.8	-	-	29.8	-	29.8	-	29.8	-	29.8	-	29.8

The precipitate will be washed in a mix of water and IPA to remove trace TTIP that is soluble in organics. The calculations for the mixing and suspension tank, MT-4, are found in Appendix A.4.3. MT-4 is an INDCO SST-300 tank with a volume of 300 gallons. The impeller diameter is 0.38 m, operating at 250 RPM. The power required to run at 250 RPM using a high-shear Rushton impeller is 2.5 kW. Each wash and suspension cycle will occur over 15 minutes of mixing. This suspension is then pumped through the centrifuge and separated once more. The washing process is repeated three times, for a total washing and centrifugation time of approximately 12.3 hours, to ensure thorough purification before the final wet cake proceeds to the drying stage. A general diagram of the washing process can be seen in Figure 4.3.2-1.

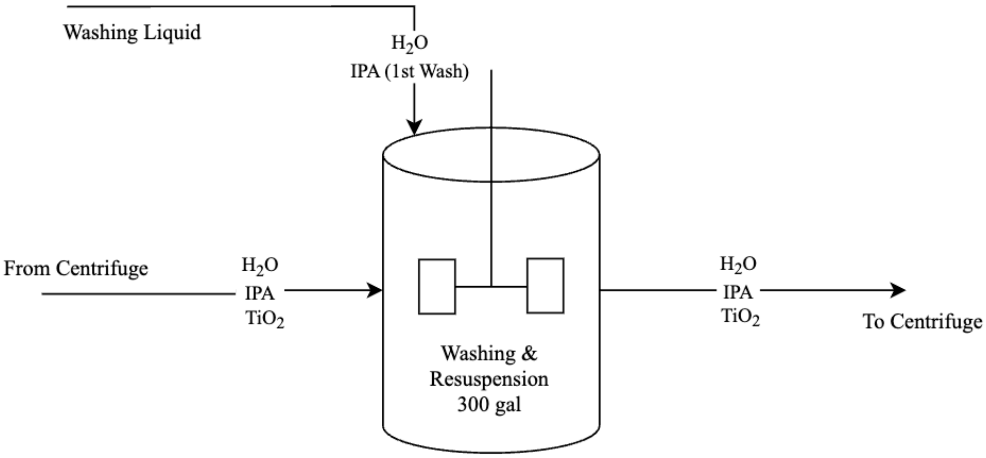

Figure 4.3.2-1: Washing Process Diagram

4.3.3. Drying & Calcining

TiO_2 is dried in the same manner as ZnO using a rotary dryer with counter-current air. The drying process takes approximately an hour to achieve a powdered product. By the time the wet cake reaches the dryer, there is a negligible amount of IPA and it no longer presents a flammability risk since it was removed during washing and centrifugation. The rotary dryer is designed to evaporate approximately 90% of the liquid content. The outlet hot air stream is vented to the atmosphere. The drum's final dimensions differ from the ZnO dryer due to different water contents. Regardless, the steps taken to find the final design reflect the different systems. All calculations are found in Appendix A.5.3.

The final design of the drum is 1.2 m in diameter, 9 m in length, 12 flights of 0.15 m radial height, and at a slope of 0.68 degrees. The heat required is 25425 kJ/hr, and the airflow is 1217 kg/hr. The inlet air temperature is 140°C and the outlet temperature is 116°C. The wet cake enters at 20°C and a dried powder exits at 100°C.

Calcination is used to further dry materials and control particle size. Much research has been done on the effects of calcination temperature and time on nanoparticle size, stability, and catalytic properties (Kim, 2021). The dried TiO_2 is calcined in a rotary kiln at 900°C for 2 hours. Our calciner is indirectly heated with natural gas. It is 4 m long and has a diameter of 0.5 m. This step removes any remaining liquid by evaporating all water that surpassed the drying step and encourages the formation of stable nanoparticle networks. At this processing time and temperature, the final TiO_2 particle size is approximately 52 nm, suitable for sunscreen formulation (Kim, 2021).

To determine the specifications needed for the calciner to successfully achieve calcination at 900°C, the following calculations and assumptions were made. First, the temperature of the air leaving the calciner was determined. The calciner air temp will be held at 1000°C. Any greater temperature is not necessary for this process since there is no reaction occurring in the calciner that would depend on a large differential of heat from the achieved calcine temperature; rather, we are only performing calcination. To determine the air temperature, the assumed heuristic was 1.5 number of thermal units (NTU) (Equation 4.3.3-1). Additionally, using the wet bulb temperature of the plant location in Austin, Texas, using the formula below, the exit air temperature is 243°C. These calculations can be found in Appendix A.7.

$$NTU = ln\,[\frac{T_G - T_W}{T_{G2} - T_W}] \approx 1.5 \qquad (4.3.3\text{-}1)$$

Next, the total heat required to calcine over 2 hours was determined. The total heat required is the sum of the heat needed to remove residual water from the TiO_2 leaving the dryer, and the heat required to raise the temperature of the TiO_2 from 100°C (the exiting temperature from the dryer) to 900°C. Equation 4.3.3-2 shows the calculation performed to determine the heat required to remove the residual water from the dryer step.

$$q_{H_2O,out} = \frac{kg\ H_2O\ out}{2\ hours} \cdot [C_{p,H_2O}\,(T_w - T_i) + C_{p,H_2Ovap}\,(T_{G2} - T_w) + \Delta H_{vap}] \quad (4.3.3\text{-}2)$$

The heat required to raise the temperature of the TiO_2 was found by finding the average heat capacity of TiO_2 at the feed and exit temperatures. As shown in Equation 4.3.3-3, the required heat was calculated.

$$\Delta Q = m\left(\frac{C_{p,TiO_2}@\ 100℃ + C_{p,TiO_2}@\ 900℃}{2}\right)\Delta T \quad (4.3.3\text{-}3)$$

After calcination, the TiO_2 particles cool down before they are sent to the next process. This is done by thinly spreading the solid onto a conveyor belt. Calculating the amount of time needed was done by using Equation 4.3.3-4 by treating the system as a lumped-capacitance model.

$$t = \frac{\rho c_p V}{hA} ln\,(\frac{T_f - T_\infty}{T_i - T_\infty}) \quad (4.3.3\text{-}4)$$

The area was calculated by taking the total volume of TiO_2 and assuming a thickness of 0.1 cm (0.001 m). Since no fans are being used to blow air over, a convective heat transfer coefficient (h) for natural air was used. The nanoparticles are cooled from 900°C to 30°C in an ambient air temperature of 25°C. This results in a cooling time of 30 minutes. After cooling, the TiO_2 is stored in a 10-gallon drum. It is later to be discharged for homogenous mixing with ZnO in a double cone blender at a bag dump station with a screw feeder.

4.4. Distillation of Isopropyl Alcohol

The distillation column will separate the waste IPA and water from our washing steps in a continuous distillation process. The final IPA/water composition from all centrifuging steps results in a bulk 21 vol% (6 mol%) IPA solution. This is stored in ST-4 before sending directly to the column. This feed is introduced at a temperature of 25°C and 1 atm. Our distillation column produces 50.4 L/hr of IPA-rich distillate (tops) and 149 L/hr of water-rich bottoms. As IPA is often sold by volume percentages, the values above are restated into volume terms with a top product of 81 vol% IPA and the bottoms contain 0.0005 vol% IPA. The tops are then sent to be recycled into our washing step, and the excess will be diluted and sold as 70% IPA. The bottoms are diluted enough to be sent to the sewer. The column consists of 6 stages with a diameter of 0.25 m. There is 5 stages of packed separation plus the reboiler. It utilizes Intalox saddle packing with a size of 25 mm saddles. The Height Equivalent to Theoretical Plate (HETP) is based of a rule of thumb where HETP is the equivalent to column diameter. This rule of thumb can only be used for small diameter columns, for which our diameter, 0.25m, applies (Fernandes Mendes, 2011). The total height of packing is 1.25m. The bottom holding volume is ten times the boil-up rate, while the top section has extra height added above the stage that is equivalent to one diameter length. The overall column height is determined to be 2.6 meters (Appendix A.8).

When doing the McCabe-Thiele analysis on a column with these product and feed purities, the theoretical number of stages was 4 (Figure 4.4.1). To have more than sufficient space for separation, our final design is 6 stages: 5 packed stages and a reboiler.

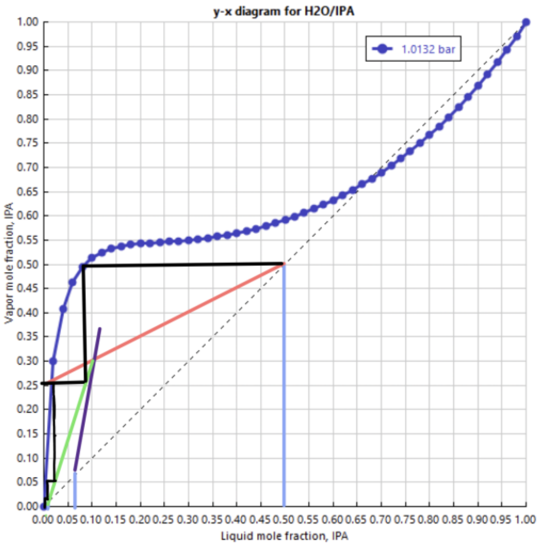

Figure 4.4.1: McCabe-Thiele Diagram of IPA & Water system at 1 atm

To ensure a continuous feed of IPA/water into the distillation column, and prevent the column from running dry, there is a storage tank, ST-4, that holds 8.5x the daily distillation feed requirement, equivalent to 17x the daily amount of post-washing liquid. ST-4 holds 8181 gallons of IPA and water, and it has a maximum holding volume of 10000 gallons (Convault, 2024). The distillation column will run continuously for fourteen days and then shut down for fifteen days to have the storage tank refilled (Appendix A.8.3). This was determined based on the maximum amount of IPA we want to store on-site and the consumption rate of our column.

From Aspen simulations, the temperature profile across the column indicates a gradual decrease from the reboiler to the condenser, ensuring efficient phase separation. The profile can be found in Figure 4.4.2.

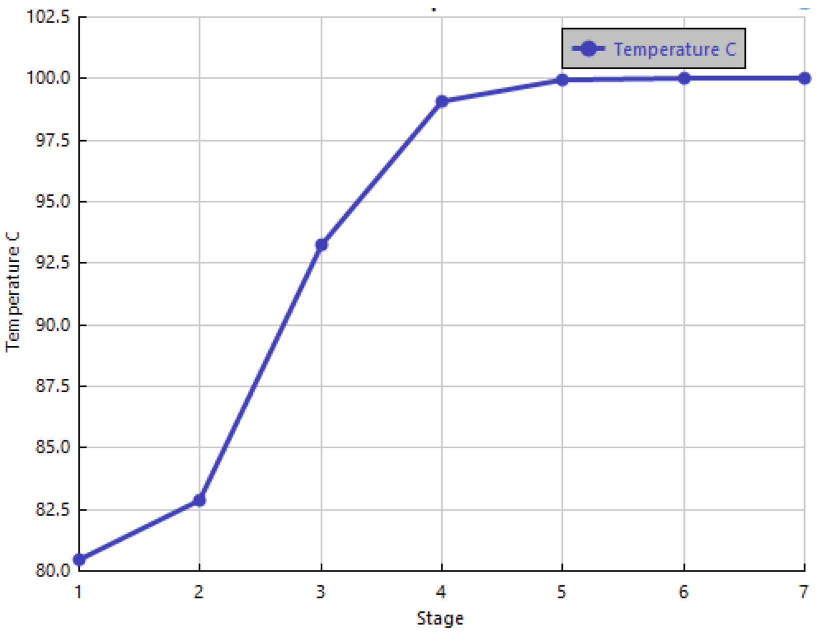

Figure 4.4.2: Temperature Profile Across Distillation Column

The pressure drop across the column is minimal. The reboiler heat duty is 50.7 kW, requiring a heat exchanger area of 0.63 m^2. The reboiler utilizes steam at 7 bar at 170°C, ensuring sufficient heat input for phase change. The condenser heat duty is -34.4 kW. Using cooling water at 30°C, this requires 0.77 m^2 of heat transfer area. These calculations can be found in Appendix A.8.1 and Appendix A.8.2. This design ensures efficient and cost-effective separation of IPA and water, maintaining product purity and operational stability.

A reflux drum is placed after the condenser at the top of the distillation column. This drum accumulates liquid from the condenser before it gets split into the reflux and the product streams. This prevents fluctuations in the flow rate leading back into the column. A heuristic states that a reflux drum is oriented horizontally and has a hold-up time of 300 seconds, or 5 minutes, to be filled halfway (Peters et al., 2003). To calculate the dimensions, Equation 4.4.4-1 was used from Silla (2003).

$$V_{total} = \frac{\pi D^2 L}{4} + 2 f_{HV} D^3 \qquad (4.4\text{-}1)$$

Length-to-diameter ratios can vary from 2.5 to 6. Due to the small amounts of liquid being held, a ratio of 2.5 was used. The factor f_{HV} comes from the geometry of the vessel head. The reflux drum is low-pressure and therefore will be using a torispherical head. The value for f_{HV} is 0.0778. The final design of the reflux drum is 0.1016 m (4 in) in diameter and 0.254 m (10 in) in length

4.5. Sunscreen Formulation & Emulsion

The final block of the overall process is combining the different ingredients. The final sunscreen is a water-in-oil (W/O) emulsion, which involves several blending steps. The metal oxides are combined in a double-cone blender. The now-blended powder is sent to the oil phase mixing. This step adds tridecyl salicylate, styrene/acrylates copolymer, glyceryl stearate, and capric/caprylic triglyceride to the powders. Simultaneously, water and glycerin are mixed together to create the aqueous phase. Both phases are then sent to an emulsion tank to create the final sunscreen. The PFD for this block can be found in Figure 5.2.4

4.5.1. Powder Blending

Once the TiO_2 and ZnO powders are dry, cooled, and collected in storage drums, they are fed via a bag dump station and screw feeder to a powder blender. Here, they are mixed homogeneously before being incorporated into the emulsion. Several powder blender types exist, but the best option would be a double-cone blender. Double-cone blenders are less power-intensive, prevent agglomeration, and are commonly used in the cosmetic industry. The dry volume for one batch is 23.1 L of powder, composed of 89.3 kg of ZnO and 29.8 kg of $TiO_{2.}$ One batch is made per day of operation, and operation occurs over 333 days to meet the production scale. Figure 3 shows the ROSS DCB-1 double-cone blender appropriate for this mixing step. The DCB-1 model was chosen since it has the fitting working capacity for the dry volume of powders produced per batch. It has a working volume of 28 L, operates at 2 HP (1.5 kW) and 20 RPM, and will be mixed for 10 minutes.

Figure 4.5.1: Double Cone Blender from ROSS

(https://www.mixers.com/products/tumble-blenders/double-cone-blender/)

4.5.2. Aqueous Phase Mixing

After the powders are dry-blended, the process of making the sunscreen lotion begins. The lotion is an emulsion of an aqueous phase and an oil phase. The aqueous phase is 357.6 kg of water and 29.8 kg of glycerin. Glycerin is an emollient that adds moisture to the skin. The volume of the solution is 381 L or approximately 100 gallons. The aqueous phase is stirred in a mixing tank, MT-5. MT-5 is an INDCO SST-150 tank with a volume of 150 gallons. MT-5 has a diameter of 0.97 m with an impeller diameter of 0.32 m. Calculations for the mixing parameters are listed in Appendix A.9.1. The aqueous phase will be mixed for 15 minutes at 60°C. To mix at 300 RPM with a pitched-blade impeller, 470 W of power is necessary.

4.5.3. Oil Phase Mixing

The oil phase consists of all other inactive ingredients and the mineral oxides. The solution is composed of 11.9 kg of tridecyl salicylate, 6.0 kg of styrene/acrylates copolymer, 29.8 kg of glyceryl stearate, 29.8 kg of capric/caprylic triglyceride, 89.3 kg of ZnO, and 29.8 kg of TiO_2. These ingredients were chosen due to their skin benefits and lack of fragrance. The amount of each ingredient is based on Pawlowski & Petersen-Thiery (2020). More specifically, glyceryl stearate was chosen as an emulsifier because it allows for a W/O emulsion, which is preferred in cosmetics.

The liquid volume is 116 L or approximately 30.6 gallons. The mixing tank for the oil phase, MT-6, is an INDCO SST-38 tank with a volume of 38 gallons. The diameter of MT-6 is 0.58 m. The diameter of the impeller is 0.19 m. Using the calculations in Appendix A.9.2, the rotation speed and power were determined by mixing the oil phase for 15 minutes at 60°C with a pitched blade impeller. The rotation speed is 500 RPM and requires 234 W of power.

4.5.4. Emulsion Mixing

As aforementioned, this sunscreen will be a W/O emulsion. This is more beneficial than an O/W emulsion since it provides more shelf stability, is smoother, waterproof, and less susceptible to pH change with the use of mineral oxides, unlike O/W emulsions. Specifically, glyceryl stearate has a hydrophilic-lipophilic balance of 3.6 and is non-ionic, which qualifies as a W/O emulsifier. The aqueous and oil phases, from MT-5 and MT-6 respectively, are charged to a mixting tank (MT-7) at 60°C with a final composition found in Table 4.5.1 from Pawlowski & Petersen-Thiery (2020).

Table 4.5.1 Final sunscreen composition by weight percent

Ingredient	**w/w%**
ZnO	15
TiO_2	5
Water	60
Glycerin	5
Capric tryglyceride	5
Glyceryl stearate	5
Tridecyl salicylate	2
Dimethicone	2
Styrene/acrylate copolymer	1

For 20 minutes, the solution is mixed with a high shear impeller, which gradually heats the mixture to 80°C. After this process, the high shear impeller is replaced with an anchor impeller until the emulsion cools to 35°C, which takes about 5 hours. The total volume of solution is 497 L or 111 gal. MT-7 is an INDCO SST-200 tank with a volume of 200 gallons and a diameter of 0.97 m. This volume is one batch of sunscreen. One batch is made per day of operation to meet our production scale.

For high shear mixing, the Ross Model 575 Batch High Shear Mixer was chosen. This mixer has a power of 75 HP (56 kW), operates at 1200 RPM, and has a diameter of 1/3 of the tank, at 32 cm. This impeller is featured in Figure 4.5.2. Heat transfer is discussed in section 4.6.4 and Appendix A.1.

Figure 4.5.2: Ross Model 575 Batch High Shear Mixer

(https://cdn.mixers.com/Specifications/500%20Series%20Spec%20Sheet%20%202022.pdf)

After mixing with the Ross Model 575 Batch High Shear Mixer for 20 minutes in MT-7, the high shear mixer is switched to an anchor impeller in MT-7. The anchor impeller has a diameter of 90% of the tank since it pulls the emulsion from the tank walls to encourage cooling. The diameter is 0.87 m. Using the calculations in Appendix A.9.3, the power required is 300 W to operate at a nominal low mixing speed of 30 RPM. The emulsion will be removed by a positive displacement pump ideal for higher viscosity fluids and sent to storage where it will be bottled at a different facility.

4.6. Ancillary Equipment

Storage tank capacities were determined by the assumption that 30 days worth of raw material would be stored on-site. Specifications for each storage tank are provided in Table 4.6.1. All storage tanks, besides ST-1, are storing a liquid. For ST-1, our ZNH is delivered in a packaged box, so there is no storage tank needed, but a storage pallet or area is necessary. Our ZNH is labeled as a storage tank for consistency with the other raw materials.

Table 4.6.1 Storage Tank Specifications

Storage Tank	**Purpose**	**Size (L)**	**Size (Gal)**	**Quantity**
ST-1	ZNH	-	-	1
ST-2	NaOH	9464	2500	1
ST-3	TTIP	3785	1000	1
ST-4	Washing Waste for Distillation	9464	2500	1
ST-5	IPA for Washing	18927	5000	1
ST-6	Tridecyl Salicylate	454	120	1
ST-7	Glyceryl Stearate	1249	330	1
ST-8	Capric/Caprylic Triglyceride	1249	330	1
ST-9	Glycerin	909	240	1
ST-10	Styrene Acrylate Copolymer	265	70	1
ST-11	Dimethicone	265	70	1

Centrifugal pumps were chosen to transport liquid throughout our entire process. They operate at 70% efficiency and handle various flow rates, all of which are on the lower end, but within the capacity for centrifugal pumps. For flows that are small in volume (Dimethicone, ST-11) and materials that are waxy (Glyceryl Stearate, ST-7), we have operators manually transferring these materials. There are no significant hazards associated with these materials (Millipore Sigma, 2024; Parchem, 2017).

Table 4.6.2 Pump Specifications

Pump	**Description**	**Amount of Material (L/min)**
P1	Water for $Zn(NO_3)_2$ 6 H_2O preparation	143
P2	NaOH Feed	15
P3	$Zn(NO_3)_2$ $6H_2O$ Feed to Batch	122
P4	Batch effluent	139
P5	Washing Water (ZnO)	58
P6	Resuspended ZnO to C-1	58
P7	Water feed (TiO_2 reactor)	1
P8	TTIP feed	0.4
P9	TiO_2 to MT-3	1
P10	MT-3 to centrifuge	53
P11	Washing Water (TiO_2)	47
P12	Resuspended TiO_2 to C-1	42

Pump	Description	Amount of Material (L/min)
P13	ST-4 to Distillation	48
P14	Distillation Reflux	1
P15	ST-5 to wash	22
P16	ST-6 to oil mixing	1
P17	ST-8 to oil mixing	2
P18	ST-9 to aqueous mixing	2
P19	Water to aqueous mixing	26
P20	Oil Mixing Effluent	5
P21	Aqueous Mixing Effluent	26
P22	Emulsion Mixing Effluent	31

4.6.1. Zinc Oxide Reactor Heating Equipment

In the synthesis of ZnO, the starting reagents must be heated before the reaction. Specifically, aqueous sodium hydroxide is heated from room temperature (25°C) to 90°C inside the reactor before adding the zinc nitrate solution. This heating process is achieved using a warming jacket supplied with steam at 3 bar. The heat energy required to raise the temperature of the sodium hydroxide solution is calculated using the specific heat formula for a batch process shown in Equation 4.6.1-1, resulting in a total power demand of 49.7 kW.

$$Q = \frac{mc_p \Delta T}{t} \quad (4.6.1\text{-}1)$$

To achieve this heating within 30 minutes, the steam flow rate must be maintained at 82.7 kg/h, with a required jacket surface area of 0.44 m². Calculations can be found in Appendix A.10.

Once the aqueous sodium hydroxide reaches 90°C, the zinc nitrate solution is gradually added to the reactor while stirring for 13.2 hours. As this reaction is endothermic, continuous heat input is required to maintain the reaction temperature at 90°C. Using the same heat transfer calculations as before, the required constant heat supply is 3.8 kW throughout the reaction. To achieve this, the necessary steam flow rate is 6.4 kg/h.

4.6.2. *Titanium Dioxide Heating Equipment*

The synthesis of TiO_2 is an exothermic reaction, requiring a cooling jacket to maintain a reaction temperature of 65°C. During the reaction, 1.4 kW of heat is generated, necessitating a cooling water flow rate of 79.6 kg/h. The water enters the jacket at 30°C and exits at 45°C. The jacket's required surface area, 0.03 m², was determined using the specific heat formula for a continuous process, Equation 4.6.2-2, and the overall heat transfer equation, Equation 4.6.2-3.

$$\dot{Q} = \dot{m} \ c_p \Delta T \quad (4.6.2\text{-}2)$$

$$Q = UA\Delta T_{lm} \quad (4.6.2\text{-}3)$$

4.6.3. Aqueous and Oil Phase Warming Jackets

For both the aqueous and oil phases, the solution must be heated from room temperature (25°C) to 60°C during a 15-minute mixing process. Using the same warming jacket calculations as before, but adjusting for varying heat capacities and masses, the steam pressure is maintained at 3 bar. The aqueous phase requires 60.9 kW of heat, with a steam flow rate of 101.3 kg/h and a jacket area of 0.30 m^2. Additionally, the oil phase requires 3.3 kW of heat, with a steam flow rate of 5.5 kg/h and a jacket area of 0.22 m^2. Once both phases are properly mixed and heated, they are transferred to the emulsion tank.

4.6.4. Emulsion Cooling Jacket

The high shear mixer in the emulsion tank generates 55 kW of energy, which is assumed to be entirely converted into heat. Jacketing surface area requirements to entirely counteract the heat produced during the 20-minute mixing process and maintain the tank at 60°C exceed the surface area available in the mixing tank. Therefore, a cooling jacket is used to partially counteract the heat produced from mixing by allowing the mixture to steadily increase in temperature from 60°C to 80°C during the total mixing time. This is a reasonable process since heating the mixture to 80°C has no reported effect on the quality of the product and allows the required jacketed surface area to be within the area provided by the tank. Using this process, the required cooling water flow rate is 1,123,000 kg/h, entering at 30°C and exiting at 45°C with a jacket surface area of 2.3 m^2.

Once the mixing process is completed, the impeller is replaced with an anchor impeller, and the solution is cooled from 80°C to 35°C using the same cooling jacket, but with a different cooling water flow rate. The required heat transfer to the cooling jacket was calculated by determining the forced convection coefficient inside the tank and applying it to the heat transfer equation. The heat transfer coefficient was determined using the Reynolds number previously calculated for emulsion mixing (15,000), a Prandtl number of 2.8, and an assumed thermal conductivity equivalent to that of water, as the emulsion is primarily water.

The Nusselt number was calculated using a literature-based correlation for stirred tanks with paddle mixers (Daza et al., 2019). Although this may not be a perfect match for the exact flow in our mixing tank, it provides a reasonable approximation for the heat transfer coefficient. The resulting Nusselt number was 309, yielding a convective heat transfer coefficient of 188.6 $W/m^2 \cdot K$. Based on this, the total heat energy to be removed is 19.5 kW. To achieve this cooling within 5 hours, a flow rate of 223,800 kg/h of cooling water, entering at 30°C and exiting at 45°C, is required. The exit temperature of 45°C is sufficient for pumping to storage since it will be less viscous and capable of flowing via a positive displacement pump.

4.7. Safety, Health, & Environmental Concerns

The synthesis of nanoparticles involves the use of various chemicals that present a range of hazards, as outlined in Table 4.7.1, which specifies the hazard statements for each reactant and product. Notably, TTIP and IPA are classified as flammable materials. To mitigate the associated risks, all equipment, piping systems, and storage vessels will be appropriately bonded and grounded to prevent static discharge. Additionally, fireproofing measures will be implemented on all pipe racks that transport these materials to further reduce the potential for fire hazards.

Vapor detectors will be installed at strategic locations within the facility to continuously monitor for potential leaks. These detectors will be integrated with an automated alarm system that will activate in the event of a leak, ensuring prompt response actions. In terms of toxicity, TTIP, IPA, and ZNH are considered to present mild health risks. To address these concerns, all personnel involved in handling these substances will be required to wear appropriate personal protective equipment (PPE).

Furthermore, all operations will be conducted with continuous airflow monitoring systems to ensure proper ventilation, given that processing spaces will have a pressure differential to remove fumes. Spill containment measures will be in place, including dedicated spill kits containing absorbent materials and neutralizing agents tailored for the specific chemicals involved. Emergency eyewash stations and safety showers will be strategically located throughout the facility, ensuring rapid access in the event of exposure.

Table 4.7.1 Hazards of Reactants and Products of Mineral Oxide Synthesis

Chemical	**Hazard Statements**	**Threshold Limits**	**SDS Source**
TTIP	Flammable liquid (Cat 3) Serious eye damage/eye irritation (Cat 2) Specific target organ toxicity - single exposure (Cat 3)	Not available	https://www.fishersci.com/store/msds?partNumber=AAA1370322&productDescription=TITNM+IV+ISOPROPOXID+100G&vendorId=VN00024248&countryCode=US&language=en
TiO_2	Not hazardous	For TiO_2 nanoparticles (1-150 nm): OSHA TWA: 15 mg/m^3	https://www.sigmaaldrich.com/US/en/sds/aldrich/718467?userType=undefined
IPA	Flammable liquids (Cat 2) Eye irritation (Cat 2A) Specific target organ toxicity - single exposure (Cat 3)	ACGIH TWA: 200 ppm ACGIH STEL: 400 ppm NIOSH TWA: 400 ppm OSHA TWA: 400 ppm	https://www.sigmaaldrich.com/US/en/sds/SIAL/W292912?userType=undefined

Chemical	**Hazard Statements**	**Threshold Limits**	**SDS Source**
ZNH	Oxidizing solid (Cat 2) Acute toxicity - oral (Cat 4) Skin irritation (Cat 2) Eye irritation (Cat 2A) Specific target organ toxicity - single exposure (Cat 3) Acute aquatic hazard (Cat 1) Chronic aquatic hazard (Cat 2)	Not available	https://www.sigmaaldrich.com/US/en/sds/sigald/228737?userType=undefined
NaOH	Skin corrosion (Cat 1) Serious eye damage (Cat 1) Acute aquatic toxicity (Cat 3)	ACGIH C: 2 mg/m^3 OSHA PEL: 2 mg/m^3 NIOSH PEL: 2 mg/m^3	https://www.columbuschemical.com/MSDS/SDS/Sodium%20Hydroxide%2025%25%20(w-w)%20Food%20Grade%209642.pdf
$Na(NO_3)_2$	Oxidizing solids (Cat 2) Eye irritation (Cat 2A)	Not available	https://www.fishersci.com/content/dam/fishersci/en_US/documents/programs/education/regulatory-documents/sds/chemicals/chemicals-s/S25558B.pdf
ZnO	Acute aquatic hazard (Cat 1) Chronic aquatic hazard (Cat 1)	ACGIH TWA: 2 mg/m^3 ACGIH STEL: 10 mg/m^3 NIOSH TWA: 5 mg/m^3 OSHA TWA: 5 mg/m^3	https://www.sigmaaldrich.com/US/en/sds/sigald/14439?userType=undefined

Referring to the reactive hierarchy of control, we have implemented inherent procedural controls by selecting less hazardous materials for the TiO_2 synthesis process. A commonly used and cost-effective method involves the reaction of titanium tetrachloride with water, but titanium tetrachloride presents significantly greater hazards due to its high reactivity, the formation of undesirable byproducts, and the severity of associated risks (Fisher Scientific, 2023; Fisher Scientific, 2024). Specifically, titanium tetrachloride is much more reactive than

TTIP. When titanium tetrachloride comes into contact with water, it reacts violently, releasing substantial heat, which can lead to thermal burns or potentially ignite a fire. In contrast, TTIP exhibits a far milder reaction and is significantly less exothermic in comparison. Furthermore, unlike the reaction with TTIP, which produces IPA and TiO_2, the use of titanium tetrachloride generates hydrochloric acid as a byproduct. Hydrochloric acid is highly corrosive and presents significant risks, including chemical burns and severe damage to equipment. It can rapidly corrode metals and degrade concrete, which would necessitate more stringent design considerations and increase the overall operational costs of the plant. Additionally, when comparing the hazards of IPA and hydrochloric acid, while both chemicals present unique risks, hydrochloric acid is far more hazardous in terms of respiratory toxicity, environmental impact, and potential harm to aquatic ecosystems. As a result, we have opted for the less hazardous reaction pathway using TTIP.

In terms of environmental impact, titanium tetrachloride is considerably more hazardous than TTIP. The volatility of titanium tetrachloride contributes to air pollution and poses a substantial risk to surrounding ecosystems. Upon contact with water, titanium tetrachloride rapidly hydrolyzes, creating highly acidic conditions that can be detrimental to aquatic life. Conversely, when TTIP is released into waterways, it hydrolyzes to form TiO_2, which is regarded as having low toxicity to aquatic organisms, thus mitigating environmental risks. Additionally, the concentration of IPA in our waste streams, like the bottoms product of the distillation process, is at a safe concentration for disposal to sewage, not posing a risk to aquatic life.

In the context of product formulation, the sunscreen contains nanoparticles as active ingredients. An inherently safer design choice was made by developing the product in a lotion form rather than as an aerosol. Aerosolized sunscreens pose additional hazards, particularly under elevated temperatures due to the pressurized canister. Furthermore, research indicates that inhalation of ZnO and TiO_2 particles may be carcinogenic (Skocaj et al., 2011). Therefore, we chose the lotion formulation to eliminate these risks. Although the target nanoparticle size in the sunscreen formulation is 50 nm, a distribution of particle sizes will be present. According to Khorsand (2013), nanoparticles smaller than 30 nm pose a risk of being absorbed into the bloodstream. To address these concerns and adopt a conservative approach, we will carefully control the nanoparticle size distribution. Specifically, for TiO_2, according to Kim et al. (2021), 88% of the nanoparticles produced at 900°C were 50 nm in size. It is assumed that the remaining 12% are both above and below 50 nm in size. Thus, the fraction below 30 nm is suggested to be minimal. Similarly, the distribution for ZnO post-milling had a mean of 50 nm, following a distribution curve with some particles above and below 50 nm (Storion et al., 2021). Additionally, regular laboratory sampling and testing via light scattering analysis will be conducted to monitor the nanoparticle distribution, ensuring that the proportion of particles smaller than 30 nm is negligible, thereby eliminating any potential health risks.

A significant safety concern in the production process is the generation of mineral oxide powders and the risk of dust formation. To mitigate human health risks, all operators, technicians, and engineers working on processes downstream of nanoparticle synthesis (including drying, calcining, conveyor belt operations, and loading into emulsions) will be equipped with the appropriate PPE. This includes respirators in compliance with the Occupational Safety and Health Administration (OSHA) and National Institute for Occupational Safety and Health (NIOSH) standards, with filtering components designed to protect against nanoparticles in the 30-50 nm range. Additionally, Tyvek suits, gloves, shoe covers, and hairnets will be worn and properly disposed of before leaving the workspace to prevent the accidental transfer of airborne nanoparticles outside of containment areas. Single process air with a pressure differential and HEPA filters will be used in processing rooms to ensure nanoparticles are contained and to protect employees.

To minimize the risks associated with mishandling or improper storage of chemicals during the production process, a comprehensive reactivity matrix was developed using CAMEO Chemicals (Appendix A.11). Key incompatibilities identified include reactions between IPA and sodium hydroxide, IPA and ZNH, IPA and sodium nitrate, TTIP and IPA, and ZnO and water. These combinations pose significant risks, including heat generation, flammability, and the production of hazardous gases, all of which can endanger workers, the facility, and the surrounding community. To prevent potential incidents due to improper chemical handling or storage, incompatible chemicals will be segregated and stored in designated areas. Additionally, labeling will comply with the Globally Harmonized System of Classification and Labelling of Chemicals (GHS), OSHA, and National Fire Protection Association (NFPA) standards to ensure clear and accessible hazard communication. All personnel interacting with these chemicals will undergo thorough training on their chemical reactivity, and both workers and emergency responders will be equipped with the necessary knowledge to implement the correct emergency procedures in the event of an incident.

In the event of a hazardous release scenario, an ALOHA (Areal Location of Hazardous Atmospheres) model was employed to simulate the release of IPA, leading to the formation of both a toxic vapor cloud and a flammable zone. Given that IPA is maintained on-site in substantial quantities at all times, this modeling exercise assumed a worst-case scenario. Although the IPA stored and produced on-site is 81% purity, ALOHA does not accommodate for varying concentrations, requiring the use of pure IPA for modeling purposes. This approach inherently provides a conservative estimate of the potential hazard.

To ensure a conservative assessment, release scenario parameters were selected based on guidance from Crowl & Louvar (2019). For the vessel rupture scenario, the largest diameter process pipe connected to the storage tank was identified. The pipe diameter was assumed to be 8 inches, which corresponds to a rupture resulting in the release of 20% of the cross-sectional area. The corresponding leak diameter was therefore calculated to be approximately 3.6 inches.

Additionally, conservative meteorological assumptions were applied, assuming a cool, dry, winter night with minimal atmospheric mixing and a stability class of F, consistent with poor dispersion conditions. Weather data was based on historical averages for Austin, Texas, during late December (Weather-And-Climate.com, n.d.). The threat zones for both the toxic vapor cloud and flammable area were determined using default threshold limits provided by ALOHA, as outlined in Appendix A.11. The resulting threat zone for the toxic vapor cloud is illustrated in Figure 4.7.

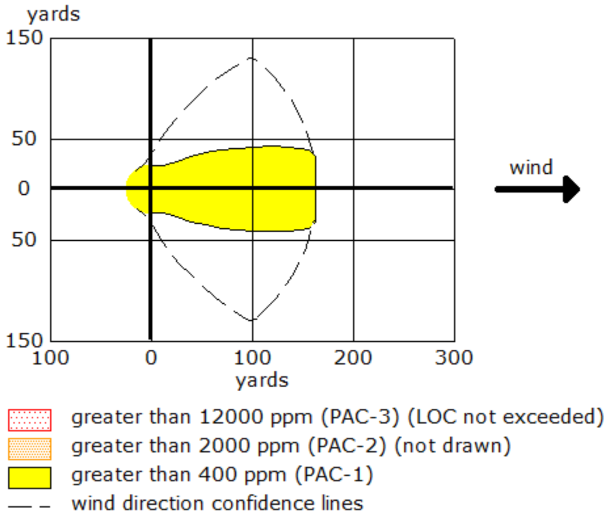

Figure 4.7: Toxic Vapor Cloud Threat Zone

The flammable area threat zones were not drawn due to the effects of near-field patchiness, making predictions less reliable. However, it was determined that the area exceeding 10% of the lower explosive limit (LEL) of IPA, equivalent to 2000 ppm, extended up to 51 yards from the release point. Notably, the upper explosive limit (UEL) was not exceeded at any location within the modeled area. To minimize the flammability risk, we will use non-sparking instrumentation, grounding and bonding, and avoid ignition sources.

Based on the toxic vapor cloud analysis provided by the ALOHA model, the extent of the cloud is approximately 162 yards. Given that the calculated concentration falls within the PAC-1 threshold, this incident would not be expected to result in significant health concerns. In toxicological and emergency response, PAC-1 represents the concentration below which a hazardous chemical is not anticipated to cause adverse health effects in the general population during short-term exposure (typically up to one hour). Therefore, the modeled exposure level suggests that the release would pose minimal health risk under the assumed conditions.

Furthermore, the chemicals involved in the emulsion of the sunscreen, including glycerin, dimethicone, glyceryl stearate, capric/caprylic triglycerides, styrene acrylates copolymer, and tridecyl salicylate, present minimal safety hazards. These ingredients are approved for cosmetic use and are incorporated into the formulation well below their respective flash points. As such, fire risks associated with these chemicals are considered negligible, further supporting the overall safety of the product from both a toxicological and fire hazard perspective.

5. Final Design

5.1. Process Description

5.1.1. Zinc Oxide Nanoparticle Synthesis

The ZnO nanoparticle synthesis is done via direct precipitation. First, our reagent solutions are prepared to the proper concentrations by feeding ZNH via a screw feeder from ST-1 and water via P1 into MT-1. Then, the NaOH solution is fed to SR-1 via P2. The zinc nitrate solution is then pumped overhead (P3) via a showerhead discharge into SR-1, following the same dropwise method used by Wu et al. (2006). ZnO directly precipitates in this reactor. The calculated specifications for these mixing and reacting tanks are in Table 5.1.1-1.

Table 5.1.1-1 ZnO Process Mixer Designs

	ZNH Preparation (MT-1)	**ZnO Reactor (SR-1)**
Temperature (°C)	25	90
Tank Size (Gal)	800	1000
Tank Material	Stainless Steel	Stainless Steel
Impeller Diameter (m)	0.5	0.61
Impeller Type	Pitched-Blade	Pitched-Blade
Mixing Time (hr)	0.5	13.2
Mixing Power (kW)	12.8	42
Mixing Speed (RPM)	190	226

The resultant ZnO slurry is centrifuged to separate our suspended solids from liquids and then sent to a resuspension tank where water washes and dilutes liquid impurities for further centrifugal separation. The slurry is pumped from SR-1 to C-1 via P4. The centrifuge will operate at a G-force of 12000xg with a nanoparticle settling velocity of 0.52 mm/s. The wet cake leaving C-1 will be sent to MT-2 for washing. The operation specifications for the washing tank can be seen in Table 5.1.1-2. This washing process is repeated three times, where the slurry is transferred back to MT-2 from C-1 via a screw feeder, to ensure all impurities are removed.

Table 5.1.1-2 ZnO Washing Specifications

	Washing (MT-2)
Temperature (°C)	25
Tank Size (Gal)	1000
Tank Material	Stainless Steel
Impeller Diameter (m)	0.61
Impeller Type	Rushton
Mixing Time (hr)	0.25
Mixing Power (kW)	7.6
Mixing Speed (RPM)	156

The ZnO slurry is dried to a powder in a rotary dryer (D-1). The slurry leaving C-1 is assumed to have enough velocity to move to the dryer. The rotary dryer specifications can be seen in Table 5.1.1-3, and the corresponding calculations are in Appendix A.5.2. This process is done in batch and will take 1 hour to completely dry. The dimensions in the table are specified to ensure the complete drying of ZnO nanoparticles.

Table 5.1.1-3 ZnO Dryer Specifications

	Dryer (D-1)
Diameter (m)	1.8
Length (m)	15
RPM	2
# Flights	18
Flight Radial Height (m)	0.23
Q_{tot} (kJ/hr)	41422
Temp Inlet Air (°C)	130
RH of inlet air (%)	0.61
Temp inlet solid (°C)	20
Air mass flow rate (kg/hr)	2468

The dried ZnO powder is larger than our desired size of 50 nm. To obtain this size, a bead mill (B-1) will be used to grind down the powder. B-1 is run at a 5:1 ratio of 5 mm hardened steel balls to the ZnO powder batch over five hours. After bead milling, ZnO is stored in a drum before being transferred to a bag dump station. It is then fed to a double-cone blender with a screw feeder to be mixed with TiO_2.

5.1.2. Titanium Dioxide Nanoparticle Synthesis

TiO_2 nanoparticle synthesis occurs via direct precipitation, where water and TTIP are mixed in a CSTR (SR-2) to produce TiO_2 and IPA. TTIP is sent from ST-3 to SR-2 via P8 while water is sent via P7. The resulting TiO_2 slurry is sent to a mixing tank (MT-3) via P9, where our process transitions from continuous to batch. The specifications for these reactors and mixing tanks are detailed in Table 5.1.2-1.

Table 5.1.2-1 TiO_2 Mixing Design Specifications

	TiO_2 CSTR (SR-2)	**TiO_2 Mixing Tank (MT-3)**
Temperature (°C)	65	25
Tank Size (Gal)	90	200
Tank Material	Stainless Steel	Stainless Steel
Impeller Diameter (m)	0.22	0.32
Impeller Type	Rushton	Rushton
Mixing Time (hr)	5	0.33
Mixing Power (kW)	93	2.1
Mixing Speed (RPM)	200	300

The separation of our TiO_2 slurry is similar to our ZnO centrifugation and washing process but with a smaller volume. The slurry is sent via P10 to C-2 for centrifugation and then sent to MT-4 for washing. The washing step is first done with 50 vol% IPA, and the following washes use only water. Because the first resuspension is different from our following steps, the stream tables in Appendix 3.2 detail how our IPA composition changes with each washing iteration. Our centrifuging will be done at the same G-force of 12000xg and will take 2.9 hrs for each cycle, resulting in a total centrifuge time of 11.6 hrs.

Table 5.1.2-2. TiO_2 Washing Specifications

	Washing (MT-4)
Temperature (°C)	25
Tank Size (Gal)	200
Tank Material	Stainless Steel
Impeller Diameter (m)	0.38
Impeller Type	Rushton
Mixing Time (hr)	0.25
Mixing Power (kW)	2.5
Mixing Speed (RPM)	250

The washed wet cake is sent to a rotary dryer (D-2) where 90% of the liquid content is evaporated. Rotary dryer specifications can be seen in Table 5.1.2-3 and the corresponding calculations in Appendix A.5.3. This process is done in batch and will take 1 hour to dry. The washing waste liquid (bulk 6 mol% IPA) is sent to a storage tank for separation with a distillation column.

Table 5.1.2-3 TiO_2 Dryer Specifications

	Dryer
Diameter (m)	1.2
Length (m)	9
RPM	2
# Flights	12
Flight Radial Height (m)	0.15
Q_{tot} (kJ/hr)	25425
Temp Inlet Air (°C)	140
RH of inlet air (%)	0.46
Temp inlet solid (°C)	20
Air mass flow rate (kg/hr)	1217

The dried TiO_2 powder is smaller than our desired nanoparticle size of 50 nm. To achieve this size, calcination is done to form crystal structures of TiO_2. Dried powder is sent to the rotary kiln (D-3) via a screw feeder. The calciner is 0.5 m in diameter and 4m in length. The powder is calcined at 900°C for two hours and removes all liquid components left in the powder to achieve a final average size of 52 nm. The calcined powder is allowed to cool on a conveyor belt and is then sent to powder blending.

5.1.3. Distillation of Isopropyl Alcohol

The waste washing liquid and IPA product are sent to a storage tank (ST-4) for distillation. The bulk liquid in the storage tank is 6 mol% IPA. The distillation column separates our IPA and water to produce an 81 vol% IPA solution as the distillate and 0.001 vol% IPA bottoms product. The bottom product is cooled and sent to the sewer, and the distillate product is sent to a storage tank for recycling into our washing step and selling the excess for profit as 70 vol% consumer-grade IPA.

Table 5.1.3-1 Distillation Column Specification

	Distillation
Stages	7
Height (m)	2.6
Diameter (m)	0.25
Pressure (atm)	1
Material	Stainless Steel
Packing Material	1-in Intalox Saddles
Reflux Ratio	2

Table 5.1.3-2 Condenser and Reboiler Specifications

	Reboiler	**Condenser**
Heat Duty (kW)	49.8	-34.4
Area (m^2)	41.7	42.3
Steam Used (kg/hr)	64.8	-
Cooling Water Used (kg/hr)	-	1973

5.1.4. Sunscreen Formulation & Emulsion

The oil and aqueous phase ingredients are prepared separately. Our metal oxide powder blend is added to the oil phase. The oil and aqueous phases are then sent to an emulsion tank.

Table 5.1.4-1 Sunscreen Mixing Parameters

	Aqueous Tank (MT-5)	**Oil Tank (MT-6)**	**Emulsion Tank (MT-7)**
Temperature (°C)	60	60	80
Tank Size (Gal)	150	38	200
Tank Material	Stainless Steel	Stainless Steel	Stainless Steel
Impeller Diameter (m)	0.32	0.19	High Shear Mixer: 0.032 Anchor Impeller: 0.87
Impeller Type	Pitched-Blade	Pitched-Blade	High Shear Mixer Anchor Impeller
Mixing Time (hr)	0.25	0.25	High Shear: 0.33 Anchor: 5
Mixing Power (kW)	0.47	0.234	High Shear: 55 Anchor: 0.3
Mixing Speed (RPM)	300	500	High Shear: 1200 Anchor: 30

5.2. Process Flow Diagrams

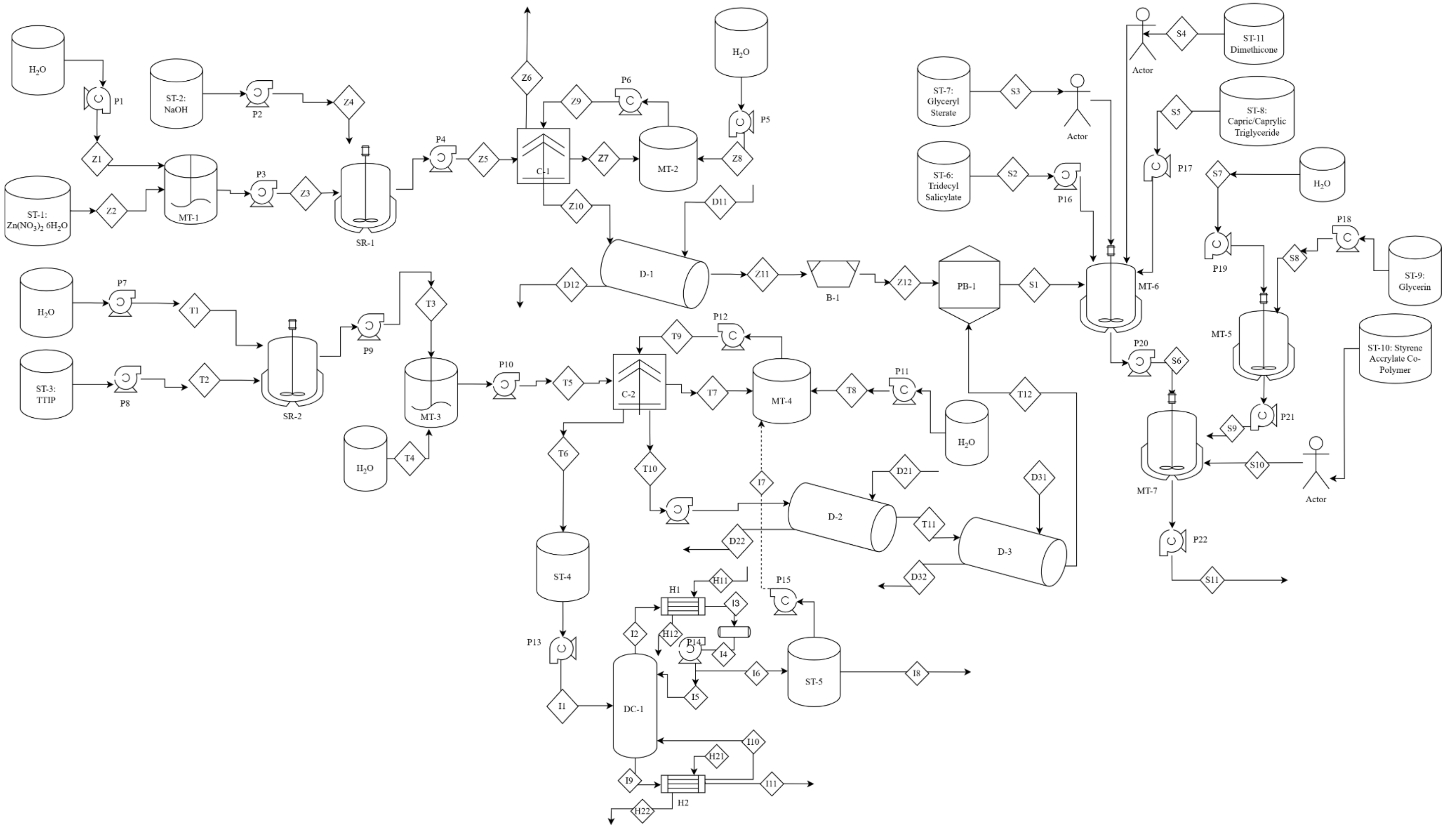

Figure 5.2.1 Complete Process Flow Diagram

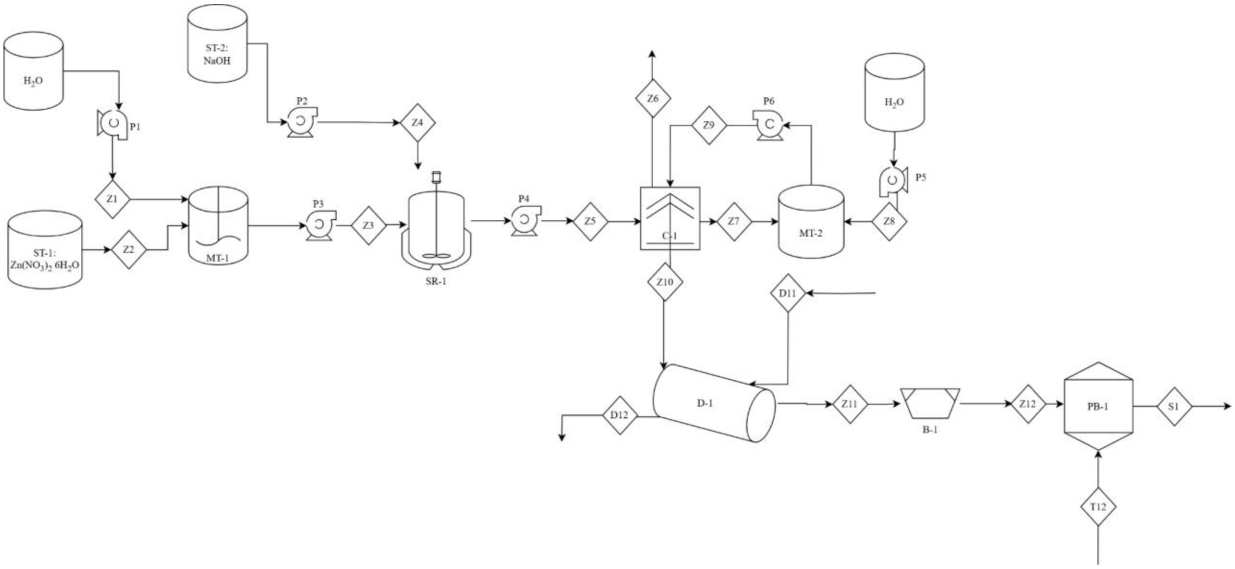

Figure 5.2.2 ZnO Process Flow Diagram

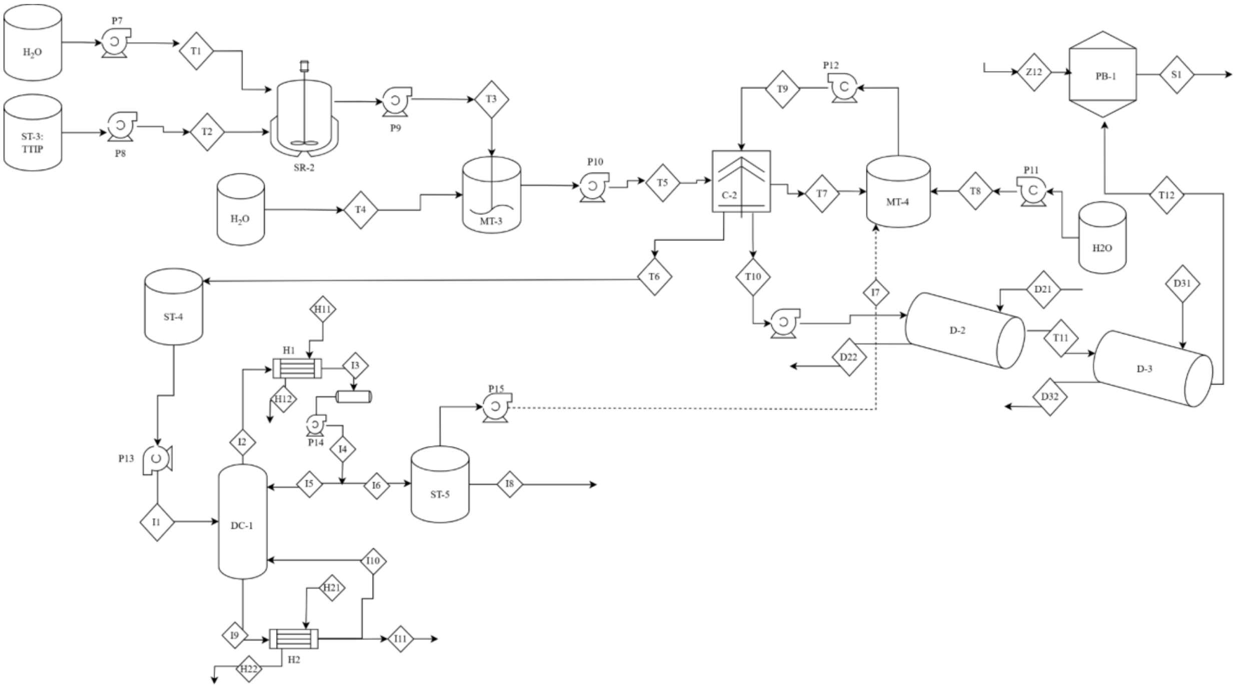

Figure 5.2.3 TiO₂ Process Flow Diagram

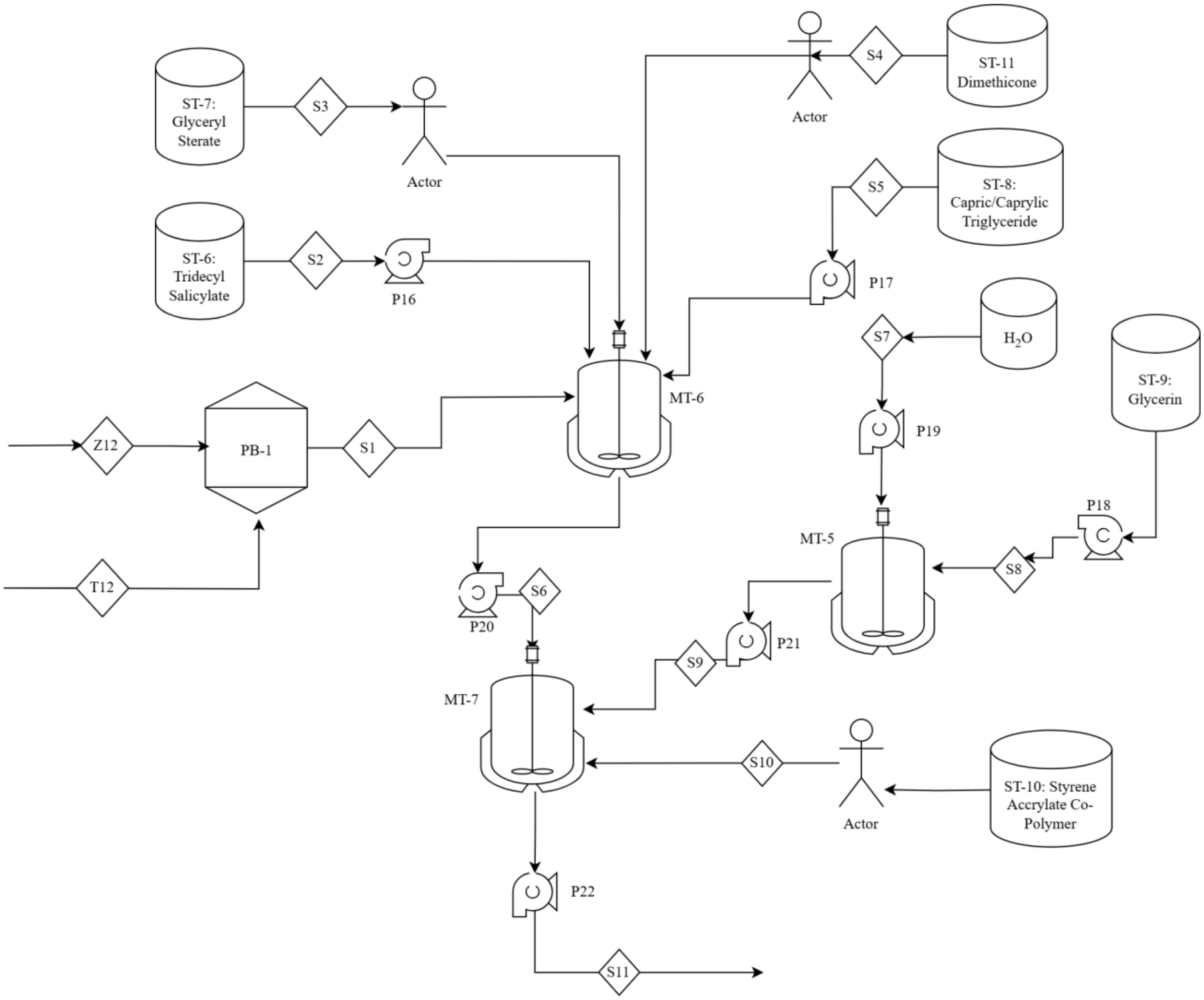

Figure 5.2.4 Sunscreen Emulsion Process Flow Diagram

5.3. Process Scheduling

The schedule in Figure 13.1, presented on the next page shows the amount of time each operation takes and the sequencing.

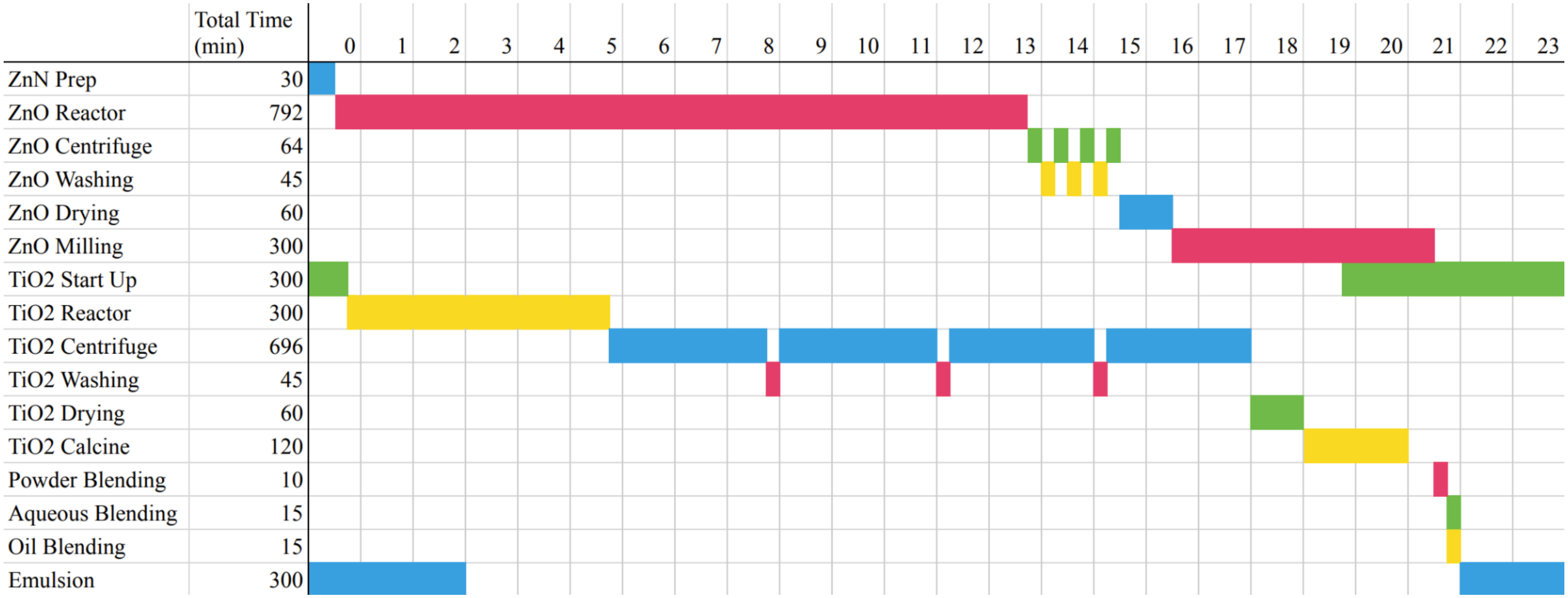

Figure 13.1: 24-hour Production Schedule

Most of the process is run in batch, and therefore sequentially, except for the TiO_2 reactor. The timing of the ZnO reactor and the startup of the CSTR for TiO_2 is set so that the reactors and their subsequent steps will be completed at the same time. This requires that SR-2 (TiO_2 Reactor) start-up to occur the day before. Centrifugation time for TiO_2 is significantly longer than for ZnO due to the difference in particle sizes. The schedule also accounts for the 30 minutes of cooling time after the calcining step before blending the powders. Aqueous and oil blending can take place simultaneously since they are independent of one another. The schedule allows for the emulsion process to begin at the end of the working day and to be cooled down and finished by the next day.

5.4. Ancillary Equipment

Our plant will store 30 days of raw materials on site. Specifications of storage tanks can be found in Table 5.4.1

Table 5.4.1 Specifications for Storage Tanks

Storage Tank	**Purpose**	**Size (gal)**	**Quantity**
ST-1	ZNH	-	1
ST-2	NaOH	2500	1
ST-3	TTIP	1000	1
ST-4	Washing Waste for Distillation	2500	1
ST-5	IPA for Washing	5000	1
ST-6	Tridecyl Salicylate	120	1
ST-7	Glyceryl Stearate	330	1
ST-8	Capric/Caprylic Triglyceride	330	1
ST-9	Glycerin	240	1
ST-10	Styrene Acrylate Copolymer	70	1

Centrifugal pumps are used throughout the process to transport liquid in our process. They have an efficiency of 70%. Table 5.4.2 shows all the pumps involved in our process.

Table 5.4.2 Specifications of Pumps

Pump	**Description**	**Amount of Material (L/min)**
P1	Water for ZNH preparation	143
P2	NaOH Feed	15
P3	Zinc Nitrate (aq) Feed to Batch	122
P4	Batch effluent	139
P5	Washing Water (ZnO)	58
P6	Resuspended ZnO to C-1	58
P7	Water feed (TiO_2 reactor)	1
P8	TTIP feed	0.4
P9	TiO_2 to MT-3	1
P10	MT-3 to centrifuge	53
P11	Washing Water (TiO_2)	47
P12	Resuspended TiO_2 to C-2	42
P13	ST-4 to Distillation	48
P14	Distillation Reflux	1
P15	ST-5 to wash	22
P16	ST-6 to oil mixing	1
P17	ST-8 to oil mixing	2
P18	ST-9 to aqueous mixing	2
P19	Water to aqueous mixing	26
P20	Oil Mixing Effluent	5
P21	Aqueous Mixing Effluent	26
P22	Emulsion Mixing Effluent	31

Heating and cooling jackets are used with mixing tanks and our stirred reactor to maintain desired process temperatures. Table 5.4.3 details the specifications of all jackets.

Table 5.4.3 Heating and Cooling Jacket Specifications

Jacket	**Description**	**Area (m^2)**	**Medium**	**Amount Used (kg/h)**
SR-1	Heating NaOH Solution	0.44	Steam	82.7
SR-1	Maintain ZnO Reaction Temperature	0.44	Steam	6.4
SR-2	Maintain TiO_2 Reaction Temperature	0.03	CW	79.6
MT-6	Heating Oil Phase	0.22	Steam	5.5
MT-5	Heating Aqueous Phase	0.30	Steam	101.3
MT-7	Maintain Emulsion Temperature	2.3	CW	1,123,000.0
MT-7	Cooling Emulsion	2.3	CW	223,800.0

5.5. Economic Analysis

The total capital cost was estimated using ratios based on the purchased equipment cost as detailed in tables 6-9 from Peters, Timmerhaus, and West. Purchased equipment was priced using current vendor numbers and pricing tables (Turton, 2012; Peters et al., 2003). Total capital costs are detailed in Table 5.5.1. The breakdown of purchased equipment can be found in Appendix B.1.

Table 5.5.1 Total Capital Cost Investment

Direct Cost	% Fixed Capital Cost	$
Purchased Equipment	0.23	$ 1,372,000
Equipment Installation	0.09	$ 537,000
Instrumentation Controls	0.06	$ 358,000
Piping	0.07	$ 418,000
Electrical Installation	0.02	$ 119,000
Buildings	0.09	$ 537,000
Yard	0.01	$ 60,000
Service	0.13	$ 776,000
Total Direct Cost		$ 4,176,000
Indirect Costs		
Engineering & Supervision	0.08	$ 477,000
Construction	0.08	$ 477,000
Contractors Fee	0.04	$ 239,000
Contingency	0.09	$ 537,000
Legal	0.01	$ 60,000
Total Indirect Cost		$ 1,790,000
Fixed Capital	1.00	$ 5,966,000
Working Capital	15% of Total Capital Investment	$ 1,053,000

Total Capital		$ 7,018,000

Total Operating Cost was determined by finding the costs associated with raw materials, waste treatment & disposal, operating labor, and utilities (Appendix B). Then, other operating costs were determined based on ratios from Figure 6-7 of Peters et al., 2003.

Table 5.5.2 Total Operating Cost

Product Cost	$/yr
Raw Materials	$ 4,700,000
Waste Treatment & Disposal	$ 247,000
Utilities: Electricity, Steam, Cooling Water, Process Water	$ 112,000
Operating Labor	$ 2,414,000
Operating Supervision (0.15 of Operating Labor)	$ 362,000
Maintenance (0.07 of Fixed Capital Investment)	$ 361,000
Operating Supplies (0.15 of Maintenance)	$ 54,000
Patents/Royalties (0.04 of Total Product Cost)	$ 0
Laboratory Charges (0.15 of Operating Labor)	$ 362,000
Total Product Cost	$ 8,612,000
Property Taxes (0.02 of FCI)	$ 121,000
Insurance (0.01 of FCI)	$ 60,000
Fixed Charges (Sum of Property Taxes and Insurance)	$ 181,000
Plant Overhead (0.6 of sum of Operating Labor, Supervision, and Maintenance)	$ 1,883,000
Total Fixed Cost	$ 2,064,000
General Expenses	
Administration (0.2 of Operating Labor)	$ 483,000

Distribution/Selling (0.15 of Total Product Cost)	$ 1,292,000
R&D (0.05 of Total Product Cost)	$ 431,000
Total General Expenses	$ 2,205,000
Total Operating Cost/COM	$ 12,881,000

Waste disposal is also included in the operating costs. The distillation bottoms' product disposal cost was calculated using commercial wastewater charge rates in Austin, TX. The stream volume is calculated for the year and then multiplied by the volume charge. There are additional charges that go towards other programs based in Austin. The cost per year for the bottom product was found to be roughly $3,520 and $12,730 for the ZnO washing stream.

The washing stream from the ZnO process should be sent to a treatment plant due to the presence of different compounds. The treatment was calculated using the wastewater treatment cost found in Peters et al. (2003) at $0.53/1000 kg. This value is multiplied by the mass of the washing stream per year. The value of this was found to be $230,136 per year. Summing these and the wastewater disposal costs totals to $246,898 per year.

Another consideration for the operational costs for the plant is labor costs. The number of workers per shift is calculated using Peters et al. (2003) with typical labor requirements based on process equipment. The total breakdown can be found in Appendix B.3.1. This number is then multiplied by a factor of 4.5 to account for all shifts with an allowance for weekends, vacations, and holidays. There will be a total of 27 operators. Employee hours were found using the required workers per shift and the number of factory working hours. Using the U.S. Bureau of Labor Statistics, the median wage of chemical plant and system operators is $50.30 in May 2023. The operator labor cost can be found by multiplying the median wage and the number of employee hours. Supervisory labor costs can be approximated to be 15% of the operator labor cost (Peters et al., 2003). Benefits are also accounted for by multiplying the total labor cost by 1.5 (Towler & Sinnot, 2021). The total labor cost is $4.16 million per year.

The plant has two main revenue streams: selling our mineral oxide sunscreen and the sale of 70% IPA (aka rubbing alcohol). The sale price is assumed to be the same every year, and our annual revenue from these streams is detailed in Table 5.5.3.

Table 5.5.3 Revenue Streams

Revenue Stream	**Amount Sold Per Year**	**Selling Price per fl. oz**	**Annual Revenue**
Sunscreen	5,200,000 fl. oz	$10	$52,000,000
70% IPA	5,074,625 fl. oz	$0.10	$507,000

The economic analysis assumes a one-year construction period followed by a 20-year operational lifespan for the plant. A federal income tax rate of 21% and a Texas franchise tax rate of 0.375%, which is applied to company revenue rather than profit, were incorporated into the financial model. Given the generally low-risk nature of the cosmetics industry, a discount rate of 10% was deemed appropriate. Depreciation was calculated using the straight-line method over the first seven years, resulting in an annual depreciation expense of approximately $1,002,623. The equipment's salvage value at the end of the 20-year period was considered negligible. Figure 5.5.1 presents the cumulative discounted cash flows over the plant’s lifetime. Both the payback period and break-even point occur in under one year, and the after-tax return on investment (ROI) is estimated at 446% annually.

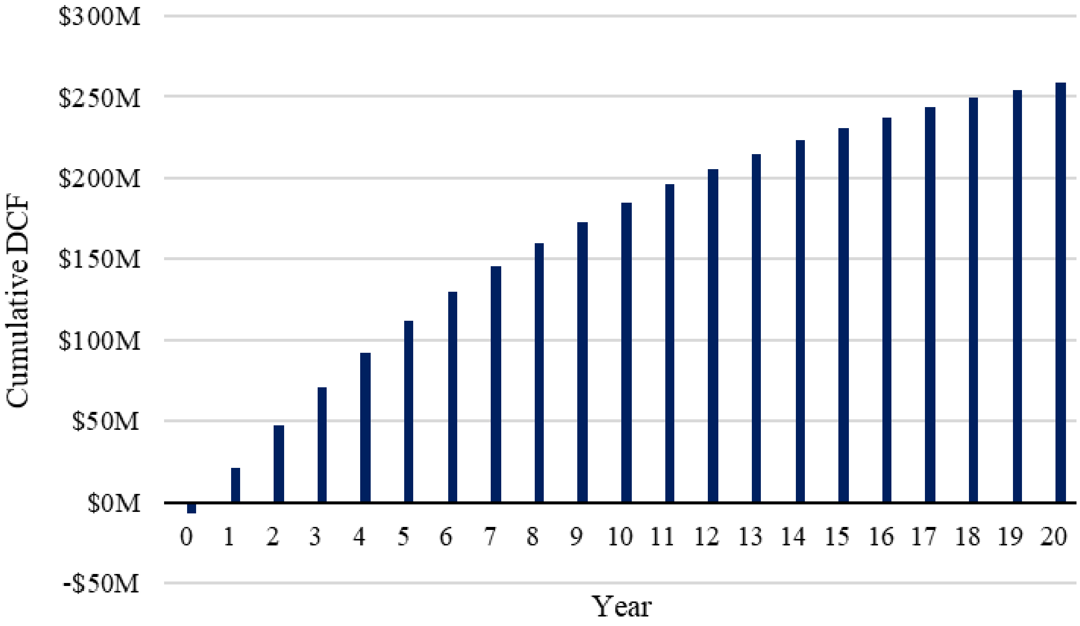

Figure 5.4.1. Cumulative Discounted Cash Flow Diagram of Total Production

6. Conclusions & Recommendation

Our project objective was to design a manufacturing facility in Austin, Texas, to produce a nanoparticle mineral oxide sunscreen. Nanoparticle mineral oxides were chosen as the active ingredient because of the UV protection they provide while still being allergy-friendly and safe for marine life. The nanoparticle size of our mineral oxides minimizes the white cast that normally appears in non-nano sunscreens. The annual production of this facility is 5,200,000 fl oz of sunscreen and is modeled after other sunscreen companies. The three main process blocks of our facility are the synthesis of ZnO nanoparticles, the synthesis of TiO_2 nanoparticles, and the blending of cosmetic ingredients and our mineral oxides to obtain our final sunscreen. Our design was created with safety and environmental considerations in mind, and reactions were chosen to minimize harm.

Our two revenue streams are the sale of sunscreen and IPA, a byproduct of the TiO_2 synthesis process. The payback period for this project is expected to be less than one year, with an after-tax ROI of 446% annually. Therefore, the team should continue with this investment.

There are possible limitations to our design due to the scale and nature of our product. We are entering a consumer market with many competitors, so annual demand is hard to predict. Sunscreen is often bought seasonally, and therefore our demand revenue streams may not be consistent throughout the year. We may need to vary the volume we produce for certain parts of the year to keep pace with demand.

For future research, we recommend testing our process in a pilot plant, as the ZnO process and TiO_2 process were all designed from literature that describes lab-scale processes. There should also be more research done on the size distribution of our nanoparticles to see if our milling and calcination steps can reach the desired size with a narrow distribution.

7. Acknowledgments

We would like to express our deepest gratitude to our technical advisor, Eric Anderson, for his guidance and advice throughout our design process. A special thanks to the University of Virginia Department of Chemical Engineering for the background and support that made this project possible.

8. Table of Nomenclature

Symbol	Definition	Unit	Section(s)
D_a	Diameter of impeller	m	4.2.1
D_T	Tank diameter	m	4.2.1
t_t	Mixing time	s	4.2.1
N_p	Power number	-	4.2.1
P	Power requirement	W	4.2.1
n	Agitation rate	min^{-1}	4.2.1
ρ	Density	kg/m^3	4.2.1
Re	Reynolds number	unitless	4.2.1
μ	Fluid dynamic viscosity	kg/(m·s)	4.2.1
V_t	Settling velocity	m/s	4.2.2
g	Gravity	m/s^2	4.2.1
$\dot{m}$	Mass flow	kg/hr	4.2.3
c_p	Heat capacity	J/(kg·K)	4.2.3
T	Temperature	K	4.2.3
Q	Heat	J	4.2.3
ΔH	Enthalpy	kJ/kg	4.2.3
C_s	Specific heat capacity of air	J/(kg·K)	4.2.3
P	Pressure	Pa	4.2.3
P_{sat}	Saturated Pressure	Bar or Pa	4.2.3
τ	Residence time	hr	4.2.3
N	Rotary dryer rotation speed	RPM	4.2.3

Symbol	**Definition**	**Unit**	**Section(s)**
D_{dryer}	Dryer diameter	m	4.2.3
L	Length of dryer	m	4.2.3
θ	Slope of dryer	deg	4.2.3
h	Convective heat transfer coefficient	$W/m^2 \cdot K$	4.3.3
A	Area	m^2	4.3.3
f_{HV}	Reflux drum head factor	Unitless	4.4
U	Overall heat transfer coefficient	$W/m^2 \cdot K$	4.6.2
ΔT_{lm}	Log mean temperature difference	°C	4.6.2

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Appendix A: Process & Equipment Calculations

A.1 Zinc Oxide Nanoparticle Material Balance

A.1.1 Production Scale:

$$5.2\ million\ oz/year$$

$$8000\ hours\ of\ operation \rightarrow 333\ days \rightarrow 1\ batch/day$$

$$\frac{5.2\ million\ units}{333\ days} \rightarrow 15615\frac{units}{day} \rightarrow 15615\ units/batch$$

$$5.72\ g\ ZnO/unit\ \ \rightarrow 15615\ units/batch \rightarrow 89\ kg\ ZnO/batch$$

A.1.2 Scale-up and Material Balances

Lab Scale:

14.87 g $Zn(NO_3)_2 \bullet 6H_2O$

4.00 g NaOH

90% yield ⟶ 3.66 g ZnO

Upscale Process:

The ratio of small-scale to large-scale reagents

$$\frac{362785.5\ g\ \ Zn(NO_3)_2\ \bullet\ 6H_2O}{14.87\ g\ \ Zn(NO_3)_2\ \bullet\ 6H_2O} = \frac{X\ g\ NaOH}{4.00\ g\ NaOH} \rightarrow 97588.8\ g\ NaOH \rightarrow 97.6\ kg\ NaOH$$

$$\frac{362785.5\ g\ \ Zn(NO_3)_2\ \bullet\ 6H_2O}{X\ mL\ H_2O} = \frac{14.87\ g\ \ Zn(NO_3)_2\ \bullet\ 6H_2O}{100\ mL\ H_2O} \rightarrow 2439721.2\ mL\ H_2O$$

$$\rightarrow 2440\ L\ H_2O$$

From material balances, need to produce 89 kg of ZnO per batch.

$$89318\ g\ ZnO\ \times \frac{1\ mol\ ZnO}{81.38\ g\ ZnO} \times \frac{1\ mol\ Zn(NO_3)_2\ \bullet\ 6H_2O}{0.9\ mol\ ZnO} \times \frac{297.49\ g\ Zn(NO_3)_2\ \bullet\ 6H_2O}{1\ mol\ Zn(NO_3)_2\ \bullet\ 6H_2O}$$

$$\rightarrow 362786.5\ g\ Zn(NO_3)_2 \bullet 6H_2O \rightarrow 362.8\ kg\ Zn(NO_3)_2 \bullet 6H_2O$$

Based on the reaction chemistry below

$$[Zn(NO_3)_2 \bullet 6H_2O] + 2NaOH \rightarrow ZnO + 7H_2O + 2NaNO_3$$

Specifically, after dissolving ZNH in water

$$Zn(NO_3)_2 + 2NaOH \rightarrow ZnO + H_2O + 2NaNO_3$$

and the 90% conversion of reagents to products, the I/O material balances are displayed in

Table A1.2-1 Material Balance

Table A.1.2-1

Material balances for feed and reactor effluent streams

Component	In (kg/batch)	Out (kg/batch)
$Zn(NO_3)_2 \bullet 6H_2O$	362.8	36.2
NaOH	97.6	9.8
H_2O	2440.0	2577.0
$NaNO_3$	0	186.6
ZnO	0	89.3

Table A.1.2-2 Stream table for zinc oxide processing.

Stream Name	Z1	Z2	Z3	Z4	Z5	Z6 - After All 3 Washes
kg/batch	2015.0	362.8	2377.8	391.0	2747.9	7526.5
Component Breakdown						
ZnO	-	-	-	-	89.3	0
ZNH	-	362.8	0	-	-	-
$Zn(NO_3)_2$	-	-	231.2	-	23.1	23.1
NaOH	-	-	-	97.6	9.8	9.8
$NaNO_3$	-	-	-	-	167.9	167.9
H_2O	2015.0	-	2146.6	293.4	2457.8	7325.7
Air	-	-	-	-	-	-

	Resuspension 1				Resuspension 2				Resuspension 3			
Stream Name	Z6	Z7	Z8	Z9	Z6	Z7	Z8	Z9	Z6	Z7	Z8	Z9
kg/batch	2642.7	105.2	2441.9	2457.8	2441.9	105.2	2441.9	2547.1	2441.9	105.2	2441.9	2547.1
Component Breakdown (kg/batch)												
ZnO	0	89.3	-	89.3	0	89.3	-	89.3	0	89.3	-	89.3
ZNH	-	-	-	-	-	-	-	-	-	-	-	-
$Zn(NO_3)_2$	23.0	0.1	-	0.1	0.1	0	-	0	0	0	-	0
NaOH	9.7	0.1	-	0.1	0.1	0	-	0	0	0	-	0
$NaNO_3$	166.9	1.0	-	1.0	1.0	0	-	0	0	0	-	0
H_2O	2443.1	14.7	2441.9	2456.6	2440.7	15.9	2441.9	2457.8	2441.9	15.9	2441.9	2457.8
Air	-	-	-	-	-	-	-	-	-	-	-	-

Table A.1.2-2 Cont.

Stream Name	Z7	Z8	Z9	Z10	D11	D12	Z11	Z12
kg/batch	105.2	2410.1	2515.3	105.2	2407.0	2422.9	89.3	89.3
Component Breakdown								
ZnO	89.3	-	89.3	89.3	-	-	89.3	89.3
ZNH	-	-	-	-	-	-	-	-
$Zn(NO_3)_2$	-	-	-	-	-	-	-	-
NaOH	-	-	-	-	-	-	-	-
$NaNO_3$	-	-	-	-	-	-	-	-
H_2O	15.9	2410.1	2426	15.9	-	15.9	0	-
Air	-	-	-	-	2407.0	2407.0	-	-

A.2 Zinc Oxide Nanoparticle Synthesis

A.2.1. Reagents Preparation

25% w/w NaOH

ρ = 1.27 g/mL

Mass of solution

$$\frac{97588.8\ g\ NaOH}{0.25} = 390352\ g\ 25\%\ w/w\ NaOH\ \rightarrow 390.4\ kg\ 25\%\ w/w\ NaOH$$

Volume of solution

$$\frac{390352\ g\ NaOH}{1.27\ \frac{g}{mL}} = 307.4\ L\ 25\%\ w/w\ NaOH \rightarrow 292.8\ L\ H_2O$$

MT-1 for prepping $Zn(NO_3)_2\ \bullet\ 6H_2O$ in solution

Considering the increase in volume due to $Zn(NO_3)_2\ \bullet\ 6H_2O$ in solution becomes $Zn(NO_3)_2$ and water.

Molar Mass of Relevant Elements

$Zn(NO_3)_2\ \bullet\ 6H_2O$ mw	297.49 g/mol
$Zn(NO_3)_2$ mw	189.41 g/mol
$6H_2O$ mw	108.08 g/mol

$$mass\ fraction\ of\ Zn(NO_3)_2\ = \frac{189.41\ g}{297.49\ g} =\ 63.67\%$$

$$mass\ fraction\ of\ H_2O\ = \frac{108.08\ g}{297.49\ g} =\ 36.33\%$$

$$362.8\ kg\ \times\ 0.6367\ =\ 231.2\ kg\ Zn(NO_3)_2$$

$$362.8\ kg\ \times\ 0.3633\ =\ 131.6\ kg\ \ H_2O \rightarrow\ 131.6\ L\ H_2O$$

Additional water needed for the solution

$$2439.7\ L\ H_2O\ (total) - 292.8\ L\ H_2O\ (from\ NaOH\ soln) - 131.6\ L\ H_2O\ (from\ ZNH)$$

$$= 2015\ L\ H_2O$$

The total volume of solution for MT-1

$$2015\ L\ H_2O + 131.6\ L\ H_2O = 2146.6\ L\ H_2O \rightarrow 567\ gal$$

Total volume needed for MT-1

$$\frac{567\ gallons}{80\%\ working\ volume} = 709\ gallons \rightarrow 800\ gallons$$

Based on nominal dimensions for an 800-gallon mixing vessel

D_T = 1.52 m

Using the rule of thumb: $3D_a = D_T$

D_a = 0.5 m

Assuming a tip speed of 5 m/s

$$\frac{5\frac{m}{s} \times 60\ sec}{\pi \times 0.5\ m} = 190\ RPM$$

Determining the density of the mixture

$$\rho = \frac{2146\ kg\ H_2O + 231.2\ kg\ Zn(NO_3)_2}{2146\ L} = 1.11\frac{g}{mL} = 1110\ kg/m^3$$

Determining the Reynolds number

Assuming a viscosity of 10^{-3} Pa s due to the high solubility of $Zn(NO_3)_2 \bullet 6H_2O$

$$Re = \frac{(0.5\ m)^2(190/60\ RPS)(1110\frac{kg}{m^3})}{10^{-3}\ Pa\ s} = 8.8 \times 10^5$$

Using a pitched blade turbine N_p = 1.1

To find power

$$1.1 = \frac{P}{(\frac{190}{60} RPS)^3 (0.5\ m)^5 (1110 \frac{kg}{m^3})} \rightarrow P = 1212\ W = 12.1\ kW$$

A.2.2 Reactor Vessel Design, SR-1

Total volume (rounding to nominal reactor size)

$$2439.7\ L \rightarrow \frac{2439.7\ L}{80\%} \rightarrow 3049.6\ L \rightarrow 805\ gallons \rightarrow 1000\ gallon\ reactor$$

With dimensions D_T = 182.9 cm and D_a = 60.96 cm

Using the equation below to determine the adequate mixing time based on the literature

$$\frac{t_{t2}}{t_{t1}} = (\frac{D_{a2}}{D_{a1}})^{\frac{11}{18}}$$

$$\frac{t_{t2}}{150\ min} = (\frac{60.96\ cm}{4\ cm})^{\frac{11}{18}} \rightarrow 792.5\ minutes \rightarrow 13.2\ hours$$

Scaling power based on volume ratio from the previous Capstone

$$V_1 = 50\ L \rightarrow P_1 = 869\ W$$

$$V_2 = 2439.7\ L \rightarrow V_1 : V_2 \rightarrow 1 : 48.8$$

$$48.8 \times 869\ W = 42407.2\ W \rightarrow 42\ kW$$

McCabe Figure 9.13

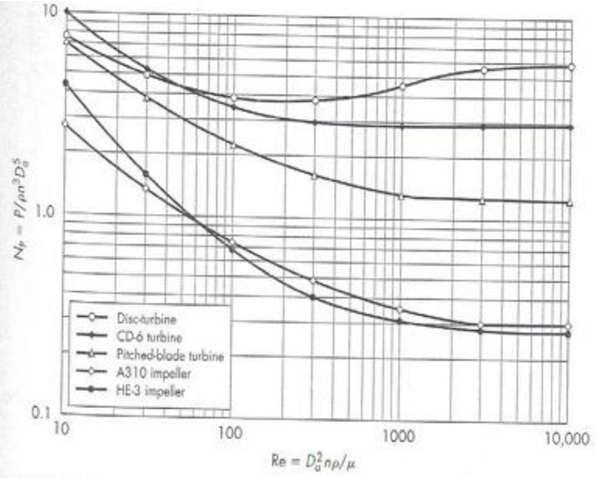


FIGURE 9.13
Power number N_p versus Reynolds number Re for turbines and high-efficiency impellers.

Holding N_p = 1.1 and a pitched blade impeller constant

$$1.1 = \frac{42407.2\, W}{\left(\frac{n}{60} RPS\right)^3 (1189\ \frac{kg}{m^3})(0.6069\ m)^5} = 226\ RPM$$

Confirming Re is turbulent

$$Re = \frac{(0.6069\ m)^2 (\frac{226}{60} RPS)(1189\ \frac{kg}{m^3})}{10^{-3} Pa\ s} = 1.65\ \times 10^6$$

A.2.3 Centrifugation Design

Settling velocity, *V_t*

$$\frac{(12{,}000)(9.81\frac{m}{s})(200 * 10^{-9} m)^2 (5600\frac{kg}{m^3} - 1000\frac{kg}{m^3})}{(18 * .001\frac{m^2}{s})} = .0012\ \frac{m}{s}$$

Separation time, *t*

$$\frac{0.5m}{0.0012\frac{m}{s}} = 41.67s$$

A.2.4 Washing and Suspension Tank

Total volume needed for the tank (the volume of soln from SR-1 and the volume of ZnO produced)

$$\frac{2474\ L}{80\%\ working\ volume} = 3093\ L = 817\ gallons \rightarrow 1000\ gallons$$

With dimensions D_T = 182.9 cm and D_a = 60.96 cm

Assuming a tip speed of 5 m/s

$$\frac{5\frac{m}{s} \times 60\ sec}{\pi\ \times 0.6069\ m} = 156\ RPM$$

Determining Reynolds number

$$Re = \frac{(0.6069\ m)^2(156/60\ RPS)(1028\frac{kg}{m^3})}{10^{-3}\ Pa\ s} = 1\ \times 10^6$$

Using a high-shear Rushton impeller to ensure suspension, $N_p = 5$

$$5 = \frac{P}{\left(\frac{156}{60}RPS\right)^3(1028\,\frac{kg}{m^3})(0.6069\ m)^5} \rightarrow 7.6\ kW$$

A.3 Titanium Dioxide Nanoparticle Material Balance

A.3.1 Production Scale

$$5.2\ million\ oz/year$$

$$8000\ hours\ of\ operation \rightarrow 333\ days \rightarrow 1\ batch/day$$

$$\frac{5.2\ million\ units}{333\ days} \rightarrow 15615\frac{units}{day} \rightarrow 15615\ units/batch$$

$$1.91\ g\ TiO_2/unit\ \rightarrow 15615\ units/batch \rightarrow 30\ kg\ TiO_2/batch$$

A.3.2 Material Balance

The required reagent amount to produce around 30 kg TiO_2

$$29825\ g\ TiO_2 \times \frac{1\ mol\ TiO_2}{79.87\ g\ TiO_2} \times \frac{1\ mol\ Ti\{OCH(CH_3)_2\}_4}{1\ mol\ TiO_2} \times \frac{284.22\ g\ Ti\{OCH(CH_3)_2\}_4}{1\ mol\ Ti\{OCH(CH_3)_2\}_4}$$

$$\rightarrow 106133.2\ g\ Ti\{OCH(CH_3)_2\}_4\ \rightarrow 106.1\ kg\ TTIP$$

The ratio of reactants (2:3 mass ratio)

$$\frac{106133.2\ g\ Ti\{OCH(CH_3)_2\}_4}{2\ g\ Ti\{OCH(CH_3)_2\}_4} = \frac{X\ g\ H_2O}{3\ g\ H_2O} \rightarrow 159{,}199.8\ g\ H_2O \rightarrow 159.2\ kg\ H_2O$$

The ratio of TTIP to water (mass ratio 2:3)

Based on reaction chemistry

$$Ti\{OCH(CH_3)_2\}_4 + 2H_2O \rightarrow TiO_2 + 4(CH_3)_2CHOH$$

Conversion is 100%

In a continuous process (producing in a time of five hours): The output is 5.96 kg TiO_2/hr. All following outputs are adjusted for this.

Table A.3.2-1

Material Balances for Feed and Effluent around the reactor (kg/batch)

Component	**In (kg/batch)**	**Out (kg/batch)**
TTIP	106.1	0
H_2O	159.2	145.6
IPA	0	89.7
TiO_2	0	29.8

Table A.3.2-2

Stream Tables for TiO_2 Synthesis and Separations

Stream Name	T1	T2	T3	T4	T5	T6 - After all 3 Washes
kg/batch	159.2	106.1	265.1	566.5	831.6	2177.0
Component Breakdown						
H2O	159.2	-	145.6	566.5	712.1	1813.4
IPA	-	-	89.7	-	89.7	-
TiO2	-	-	29.8	-	29.8	363.7
Air	-	-	-	-	-	-
TTIP	-	106.1	0.0	-	-	-

Table A.3.2-2 Cont.

	Resuspension 1					Resuspension 2				Resuspension 3			
Stream Name	T6	T7	T8	I7	T9	T6	T7	T8	T9	T6	T7	T8	T9
kg/batch	794.6	37.0	320.0	354.7	711.7	674.6	37.1	707.9	717.7	707.9	37.1	707.9	717.7
Component Breakdown													
H2O	705.5	6.6	320.0	80.7	407.3	403.4	3.9	707.9	711.8	704.5	7.3	707.9	717.7
TTIP	-	-	-	-	-	-	-	-	-	-	-	-	-
IPA	89.1	0.6	-	274.0	274.6	271.2	3.4	-	3.4	3.4	0.0	-	0.0
TiO_2	-	29.8	-	-	29.8	-	29.8	-	29.8	-	29.8	-	29.8
Air	-	-	-	-	-	-	-	-	-	-	-	-	-

Stream Name	T10	D21	D22	T11	D31	D32	T12
kg/batch	37.1	1217.0	1229.7	30.3	0.0	0.5	29.8
Component Breakdown							
H2O	7.3	-	6.6	0.7	-	0.7	0.0
TTIP	-	-	-	-	-	-	-
IPA	0.0	-	0.0	0.0	-	0.0	-
TiO_2	29.8	-	-	29.8	-	-	29.8
Air	-	1217.0	1217.0	-	-	-	-

A.4 Titanium Dioxide Nanoparticle Synthesis

A.4.1 Reactor Vessel, SR-2

Liquid volume (based on reagents):

$$106.1\ kg\ TTIP \times \frac{L}{.96\ kg} = 110.5\ L\ TTIP$$

$$159.2\ kg\ H_2O\ \times \frac{L}{1\ kg}\ =\ 159.2\ L\ H_2O$$

$$Total\ liquid\ volume\ =\ 269.7L$$

Total volume (rounding to nominal reactor size)

$$269.7\ L\ =\ 0.8 * X\ \rightarrow\ 337.125\ L\ or\ 89.1\ gal$$

Aspect ratio (reactor height to tank diameter): 1.5:1

$$h\ =\ 1.5d = 0.99\text{ m}$$

$$V\ =\ \pi d^2 h/4 \rightarrow 337\ =\ \pi d^3 * 1.5/4\ \rightarrow d\ =\ 0.66m$$

Tank diameter: D_T = 0.66 m

Impeller diameter: D_a = 0.22 m

Assuming a rotation speed of 200 RPM

$$Re =\ \frac{(0.22\ m)^2(\frac{200}{60}RPS)(984\ \frac{kg}{m^3})}{2.06 * 10^{-3}Pa\ s} = 7.68\ \times 10^5$$

Using a high-shear Rushton impeller, N_p = 5

$$5 =\ \frac{P}{\left(\frac{200}{60}RPS\right)^3\ (984\ \frac{kg}{m^3})(0.22\ m)^5} \rightarrow 93\ W$$

A.4.2 Reactor Effluent Storage Tank

540.8 L of effluent + 171.2 L of water for adequate concentration

$$\frac{712\,L}{80\%\,working\ volume} = 890\,L = 235\,gallons \rightarrow 300\,gallons$$

With dimensions D_T = 1.14m and D_a = 38 cm

Assuming a tip speed of 5 m/s

$$\frac{5\frac{m}{s} \times 60\,sec}{\pi\ \times 0.38\,m} = 250\,RPM$$

Determining Reynolds number

$$Re = \frac{(0.38\,m)^2(250/60\,RPS)(965\,\frac{kg}{m^3})}{10^{-3}\,Pa\,s} = 5.8\ \times 10^5$$

Using a high-shear Rushton impeller to ensure suspension, N_p = 5

$$5 = \frac{P}{\left(\frac{250}{60}RPS\right)^3\ (965\ \frac{kg}{m^3})(0.38\,m)^5} \rightarrow 2.8\,kW$$

A.4.3 Centrifugation Design

Settling velocity, V_t

$$\frac{(12{,}000)(9.81\frac{m}{s})(15 * 10^{-9}m)^2(4230\frac{kg}{m^3} - 965.2\frac{kg}{m^3})}{(18 * .001\frac{m^2}{s})} = 4.2 * 10^{-6}\ \frac{m}{s}$$

Separation time, *t*

$$\frac{0.5m}{4.2 * 10^{-6}\ \frac{m}{s}} = 2.9h$$

A.4.4 Washing and Suspension Tank

Total volume needed for the tank

$$\frac{712\ L}{80\%\ working\ volume} = 890\ L = 235\ gallons \rightarrow 300\ gallons$$

With dimensions D_T = 114 cm and D_a = 38.1 cm

Assuming a tip speed of 5 m/s

$$\frac{5\frac{m}{s} \times 60\ sec}{\pi\ \times 0.381\ m} = 250\ RPM$$

Determining Reynolds number

$$Re = \frac{(0.381\ m)^2(250/60\ RPS)(854\frac{kg}{m^3})}{10^{-3}\ Pa\ s} = 2.9\ \times 10^5$$

Using a high-shear Rushton impeller to ensure suspension, N_p = 5

$$5 = \frac{P}{\left(\frac{250}{60}RPS\right)^3 (854\ \frac{kg}{m^3})(0.381\ m)^5} \rightarrow 2.5\ kW$$

A.5 Rotary Dryer Design and Calculations

A.5.1 FEECO Rotary Dryer Data

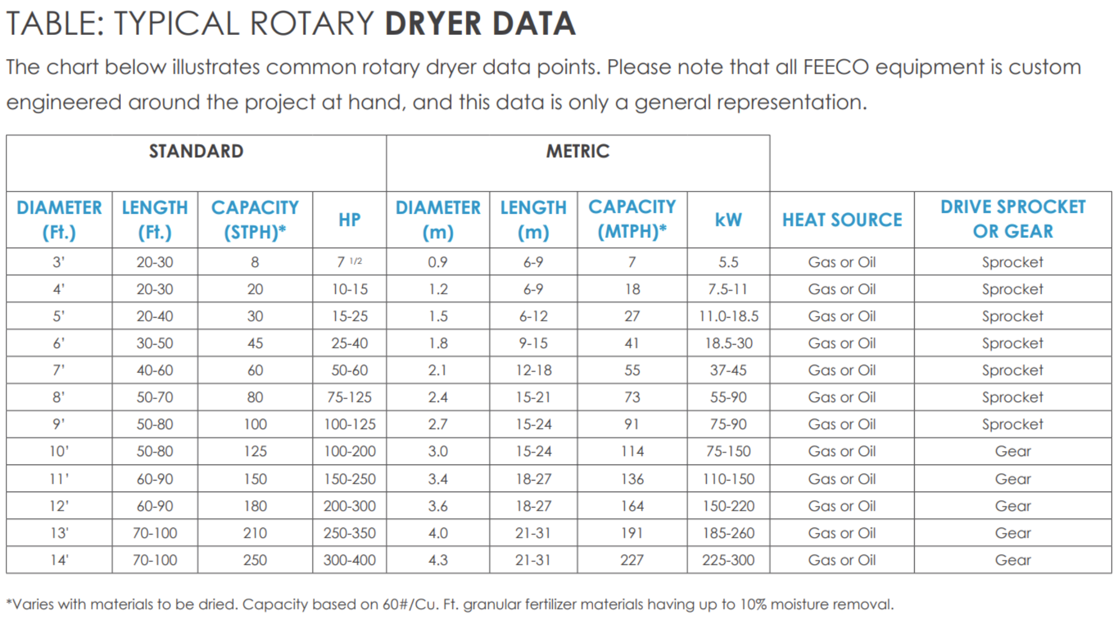


TABLE: TYPICAL ROTARY **DRYER DATA**

The chart below illustrates common rotary dryer data points. Please note that all FEECO equipment is custom engineered around the project at hand, and this data is only a general representation.

STANDARD				METRIC					
DIAMETER (Ft.)	**LENGTH (Ft.)**	**CAPACITY (STPH)***	**HP**	**DIAMETER (m)**	**LENGTH (m)**	**CAPACITY (MTPH)***	**kW**	**HEAT SOURCE**	**DRIVE SPROCKET OR GEAR**
3'	20-30	8	7 1/2	0.9	6-9	7	5.5	Gas or Oil	Sprocket
4'	20-30	20	10-15	1.2	6-9	18	7.5-11	Gas or Oil	Sprocket
5'	20-40	30	15-25	1.5	6-12	27	11.0-18.5	Gas or Oil	Sprocket
6'	30-50	45	25-40	1.8	9-15	41	18.5-30	Gas or Oil	Sprocket
7'	40-60	60	50-60	2.1	12-18	55	37-45	Gas or Oil	Sprocket
8'	50-70	80	75-125	2.4	15-21	73	55-90	Gas or Oil	Sprocket
9'	50-80	100	100-125	2.7	15-24	91	75-90	Gas or Oil	Sprocket
10'	50-80	125	100-200	3.0	15-24	114	75-150	Gas or Oil	Gear
11'	60-90	150	150-250	3.4	18-27	136	110-150	Gas or Oil	Gear
12'	60-90	180	200-300	3.6	18-27	164	150-220	Gas or Oil	Gear
13'	70-100	210	250-350	4.0	21-31	191	185-260	Gas or Oil	Gear
14'	70-100	250	300-400	4.3	21-31	227	225-300	Gas or Oil	Gear

*Varies with materials to be dried. Capacity based on 60#/Cu. Ft. granular fertilizer materials having up to 10% moisture removal.

A.5.2 Zinc Oxide Dryer Calculations

Find the mass flow of air required.

$$\dot{m}_{liq\ removed} = 15.9\ kg/hr$$

Dimensions of the drum

Diameter = 1.8 m

Length = 15 m

Air velocity = v = 0.3 m/s

$$A = \frac{\pi}{4} D^2 = \frac{\pi}{4} (1.8)^2 = 2.54\ m^2$$

$$\dot{V}_{air} = A \cdot v = 2.54 * 0.3 = 0.76 \frac{m^3}{s} = 2748 \frac{m^3}{hr}$$

$$PV = nRT$$

$$\rho_{air} = \frac{m}{V} = \frac{Pm}{RT} = \frac{(101325)(0.02897)}{(8.314)(130+273)} = 0.876\frac{kg}{m^3}$$

$$\dot{m}_{air} = \dot{V}_{air} \cdot \rho_{air} = (2748)(0.876) = 2407\frac{kg}{hr}$$

Specific heat data:

$$c_{p,dry} = c_{p,ZnO} = 495.2\frac{J}{Kg\ °C}$$

$$c_{p,liq} = c_{p,H_2O} = 4182\frac{J}{Kg\ °C}$$

Heat to raise the product temperature

$$Q_1 = \dot{m}_{dry,in} * c_{p,dry} * \left(T_{S,1} - T_{S,2}\right) + \dot{m}_{liq,in} * c_{p,liq} * (T_{G2} - T_{G1})$$

$$Q_1 = 89.3\ kg * 495.2 * (70-20) + 15.9\ kg * 4182 * (70-20) = 5535760\frac{J}{kg}$$

$$Q_1 = 5535.76\frac{kJ}{kg}$$

Heat to evaporate liquid

$$Q_2 = \dot{m}_{liq,removed} * \Delta H_v$$

$$Q_2 = 15.9\ kg * 2257\frac{kJ}{kg} = 35886\frac{kJ}{hr}$$

Total Heat Required

$$Q_{tot} = Q_1 + Q_2 = 41422.06\,\frac{kJ}{hr}$$

Calculating the heat capacity of wet air

$$C_s\,, specific\ heat\ of\ moist\ inlet$$

$$C_s = c_{p,dry\ air} + c_{p,H_2O\ vapor} * H$$

$$H, specific\ humidity$$

$$p_s\,, saturated\ pressure\ at\ T$$

$$RH = 71\%\ at\ 20°C, p_s = 2.338\ kPa$$

$$RH = ?\ at\ 130°C, p_s = 270\ kPa$$

$$e = 0.71 * (2.338\ kPa) = 1.166\ kPA$$

$$RH = \frac{actual\ vapor\ pressure\ at\ dew\ point}{vapor\ pressure\ at\ saturation} = \frac{1166\ Pa}{270000\ Pa} = 0.0061$$

$$w = \frac{e * \ R_d}{R_v * (p - e)}$$

$$R_d\,, Specific\ gas\ constant\ for\ dry\ air\ \left(\frac{J}{kg\ K}\right)$$

$$R_v\,, Specific\ gas\ constant\ for\ water\ vapor\ (\frac{J}{kg\ K})$$

$$w = \frac{1166 * 287.06}{461.5 * (101325 - 1169)} = 0.0104$$

$$w, water\ vapor\ to\ dry\ air\ mass\ mixing\ ratio$$

$$H_{in} = \frac{w}{w+1} = \frac{0.0104}{0.0104+1} = 0.0103\,\frac{kg\ H_2O}{kg\ dry\ air}$$

$$C_s = (1.005) + (1.82)(0.0072) = 1.02\,\frac{kJ}{kg\ °C} = 1020\,\frac{J}{kg\ °C}$$

Calculate air outlet temperature.

$$Q_{tot} = \dot{m}_{air}\ * C_s\ * (T_{G2} - T_{G1})$$

$$T_{G2} = T_{G1} - \frac{Q_{tot}}{\dot{m}_{air} * C_s} = 130 - \frac{41422.06}{2407 * 1020} = 116°C$$

Calculate the partial pressure of water in the air outlet stream.

$$P_{H_2O} = x_{H_2O}P_{tot} = \left(\frac{1.71}{1.71 + 82.62}\right) * 101325 = 2.049\ kPa = 0.02049\ bar$$

Calculate saturation pressure at the slurry inlet

Using Antoine’s constants from 0-30°C for water from NIST

$$log\ (P_{sat})\ = A - \frac{B}{T+C}$$

$$P_{sat} = exp\ \left(A - \frac{B}{T+C}\right) = exp\ (5.40221 - \frac{1838.675}{(20+273) - 31.737}) = 0.0232\ bar$$

Calculate the slope of the dryer

τ = 1 hour

N = 2 RPM = 120 rotations per hours

$$\tau = \frac{0.19L}{N * D * tan\,(\theta)}$$

$$\left(\frac{0.19L}{N * D * \tau}\right) = \frac{0.19(15)}{120 * 1.8 * 1} = \; 0.76$$

Flight Design

$$Number\ of\ flights = \; 3 * D[ft] = 3 * (3.28 * 1.8) = 17.7 \approx \; 18$$

$$Height\ of\ flights = \frac{1}{8} * D = \frac{1}{8} * (1.8) \approx 0.23\, m$$

A.5.3 Titanium Dioxide Dryer Calculations

$$\dot{m}_{liq\ removed} = 8.88 + 0.03 = 8.91\ kg/hr$$

Dimensions of the drum

Diameter = 1.2 m

Length = 9 m

Air velocity = v = 0.35 m/s

$$A = \frac{\pi}{4}D^2 = \frac{\pi}{4}(1.2)^2 = 1.13\ m^2$$

$$\dot{V}_{air} = A \cdot v = 1.13 * 0.35 = 0.39\frac{m^3}{s} = 1425\frac{m^3}{hr}$$

$$PV = nRT$$

$$\rho_{air} = \frac{m}{V} = \frac{Pm}{RT} = \frac{(101325)(0.02897)}{(8.314)(140 + 273)} = 0.854\frac{kg}{m^3}$$

$$\dot{m}_{air} = \dot{V}_{air} \cdot \rho_{air} = (1425)(0.854) = 1217\frac{kg}{hr}$$

Specific heat data:

$$c_{p,dry} = c_{p,TiO_2} = 848.6\frac{J}{Kg\ °C}$$

$$c_{p,liq} = w_{H_2O} * c_{p,H_2O} + w_{IPA} * c_{p,IPA}$$

$$w_{H_2O} = \frac{9.86}{9.86 + 0.03} = 0.999$$

$$w_{IPA} = 1 - w_{H_2O} = 0.001$$

$$c_{p,liq} = 0.999 * 4182 + .001 * 2682 = 4177 \ \frac{J}{Kg\ °C}$$

$$\Delta H_{v,H_2O} = 2257 \frac{kJ}{kg}$$

Heat to raise the product to the temperature

$$Q_1 = \dot{m}_{dry,in} * c_{p,dry} * \left(T_{S,1} - T_{S,2}\right) + \dot{m}_{liq,in} * c_{p,liq} * (T_{G2} - T_{G1})\ \#$$

$$Q_1 = 29.8 * 848.6 * (100 - 20) + 9.89 * 4177 * (100 - 20) = 5328000 \frac{J}{hr}$$

$$Q_1 = 5328 \frac{kJ}{hr}$$

Heat to evaporate liquid

$$Q_2 = \dot{m}_{liq,removed} * \Delta H_v$$

$$Q_2 = 8.91\ kg * 2257 \frac{kJ}{kg} = 20096 \frac{kJ}{hr}$$

Total Heat Required

$$Q_{tot} = Q_1 + Q_2 = 25425 \frac{kJ}{hr}$$

Calculating the heat capacity of wet air

$$C_s, specific\ heat\ of\ moist\ inlet$$

$$C_s = c_{p,dry\ air} + c_{p,H_2O\ vapor} * H$$

$$H, specific\ humidity$$

$$p_s, saturated\ pressure\ at\ T$$

$$RH = 71\%\ at\ 20°C, p_s = 2.338\ kPa$$

$$RH = ?\ at\ 140°C, p_s = 360\ kPa$$

$$e = 0.71 * (2.338\ kPa) = 1.166\ kPA$$

$$RH = \frac{actual\ vapor\ pressure\ at\ dew\ point}{vapor\ pressure\ at\ saturation} = \frac{1166\ Pa}{360000\ Pa} = 0.0046$$

$$w = \frac{e\ *\ R_d}{R_v * (p\ -\ e)}$$

$$R_d, Specific\ gas\ constant\ for\ dry\ air\ \left(\frac{J}{kg\ K}\right)$$

$$R_v, Specific\ gas\ constant\ for\ water\ vapor\ (\frac{J}{kg\ K})$$

$$w = \frac{1166 * 287.06}{461.5 * (101325 - 1166)} = 0.0104$$

$$w, water\ vapor\ to\ dry\ air\ mass\ mixing\ ratio$$

$$H_{in} = \frac{w}{w+1} = \frac{0.0104}{0.0104 + 1} = 0.0103 \frac{kg\ water}{kg\ dry\ air}$$

$$C_s = (1.005) + (1.82)(0.0072) = 1.02 \frac{kJ}{kg\ °C} = 1020 \frac{J}{kg\ °C}$$

Calculate air outlet temperature.

$$Q_{tot} = \dot{m}_{air} * C_s * (T_{G2} - T_{G1})$$

$$T_{G2} = T_{G1} - \frac{Q_{tot}}{\dot{m}_{air} * C_s} = 140 - \frac{25425}{1216 * 1020} = 116°C$$

Calculate the partial pressure of water in the air outlet.

$$P_{water} = x_{water}P_{tot} = \left(\frac{0.85}{0.85 + 42}\right) * 101325 = 2.14\, kPa = 0.0214\, bar$$

Calculate saturation pressure at the slurry inlet

Using Antoine's constants from 0-30°C for water from NIST

$$log\,(P_{sat}) = A - \frac{B}{T + C}$$

$$P_{sat} = exp\left(A - \frac{B}{T + C}\right) = exp(5.40221 - \frac{1838.675}{(20 + 273) - 31.737}) = 0.0231\, bar$$

Calculate the slope of the dryer

τ = 1 hour

N = 2 RPM = 120 rotations per hours

$$\tau = \frac{0.19L}{N * D * tan\,(\theta)}$$

$$\left(\frac{0.19L}{N * D * \tau}\right) = \frac{0.19(9)}{120 * 1.2 * 1} = 0.68$$

Flight Design

$$Number\ of\ flights = 3 * D[ft] = 3 * (3.28 * 1.2) = 11.8 \approx 12$$

$$Height\ of\ flights = \frac{1}{8} * D = \frac{1}{8} * (1.2) \approx 0.15\, m$$

A.6 TiO$_2$ Heat Exchanger

A.6.1 Heating Water for TiO$_2$ Reaction

$$Q = mC_p\Delta T$$

$$Q = \left(\frac{31.8\ kg}{hr} * \frac{1\ hr}{3600\ s} * 4.18\frac{kJ}{kg\ K} * \frac{1000\ J}{kJ}\right)(65 - 30\ ℃) = 1292\ W$$

Steam at 3 bar

	Water	Steam
T_{in} (C)	30	133
T_{out} (C)	65	133

ΔH_v = 2163.5 kJ/kg

Flow rate of steam

$$\frac{1.3\ kW}{2163.5\frac{kJ}{kg}} = 2.2\frac{kg}{hr} steam$$

$$\Delta T_1 = T_{1,H} - T_{2,C} = 133 - 65 = 68\ ℃$$

$$\Delta T_2 = T_{2,H} - T_{1,C} = 133 - 30 = 103\ ℃$$

$$\Delta T_{lm} = \frac{68 - 103℃}{ln\ (\frac{68}{103})} = 96℃$$

U for steam and water = 2250 W/m^{2}K

$$1292\ W = 2250\,\frac{W}{m^2K} * A * (96\ ℃) \rightarrow A = 0.006\ m^2 = 60\ cm^2$$

A.6.2 Cooling TiO_2 Effluent

Effluent temp in = 65 C

Effluent temp out = 40 C

$$Q = mC_p\Delta T$$

$$C_{p,mix} = \frac{(\frac{29.12\ kg}{hr} * 4.18\frac{kJ}{kg\ K} + \frac{17.94\ kg}{hr} * 3\,\frac{kJ}{kg\ K} + \frac{5.96\ kg}{hr} * 0.71\,\frac{kJ}{kg\ K}}{\frac{29.12\ kg}{hr} + \frac{17.94\ kg}{hr} + \frac{5.96\ kg}{hr}} = 3.39\ \frac{kJ}{kg\ K}$$

$$Q = \left(\frac{53\ kg}{hr} * \frac{1\ hr}{3600\ s} * 3.39\frac{kJ}{kg\ K} * \frac{1000\ J}{kJ}\right)(65 - 40\ ℃) = 1248\ W$$

Mass flow of water needed

Cooling water at 30 C, assuming temp out at 45 C

$$Q = mC_p\Delta T$$

$$1.25\ kW = m * 4.18\frac{kJ}{kg\ K}(15\ ℃) \rightarrow m = 72\ kg/hr$$

$$\Delta T_1 = T_{1,H} - T_{2,C} = 65 - 45 = 20\ ℃$$

$$\Delta T_2 = T_{2,H} - T_{1,C} = 40 - 30 = 10\ ℃$$

$$\Delta T_{lm} = \frac{20 - 10℃}{ln\,(\frac{20}{10})} = 14.4℃$$

U - Overall Heat Transfer Coefficient (W/(m^2K)) determined from Table 14-5 in Peters et al., 2003, and Table 12.1 in Sinnott, 2005.

U is the average of medium organics and water = 1150 W/m^2K

$$Q = UA\Delta T_{lm}$$

$$1248\ W = 1150\,\frac{W}{m^2K} * A * (14.4\ ℃) \rightarrow A = 0.1\ m^2 = 1000\ cm^2$$

A.7 TiO_2 Calciner

T_G = inlet air temperature = 1000 C = 1832 F

*Assume not humid due to the high temperature

T_w = wet bulb temperature = 26.1 C = 79.1 F

H_L = latent heat of vaporization = 2424.6 kJ/kg

T_i = initial powder inlet temperature = 100 C

Choose 1000 C for air temp since no reaction is occurring in the calciner, so it does not need to be significantly larger than the air temp

Outlet air temperature:

Heuristic NTU ≈ 1.5 (in F)

$$NTU = ln\,[\tfrac{T_G - T_W}{T_{G2} - T_W}] \approx 1.5$$

$$NTU = ln\,[\frac{1832 - 79.1}{T_{G2} - 79.1}] \approx 1.5$$

$$T_{G2} = 470\ °\mathrm{F} = 243\ ℃$$

The heat required to remove water:

$$q_{water,out} = \tfrac{kg\ water\ out}{2\ hours} \cdot [C_{p,water}\,(T_w - T_i) + C_{p,watervap}\,(T_{G2} - T_w) + \Delta H_{vap}] \text{ Eq.B-2}$$

$$q_{water,out} = \frac{15.9\ kg}{2\ hours} \cdot [4.184\frac{kJ}{kg℃}(26.1℃ - 100℃) + 1.9\frac{kJ}{kg℃}(243℃ - 26.1℃) + 2424.6\frac{kJ}{kg}]$$

$$q_{water,out} = 2.0 * 10^{4}\ \frac{kJ}{hr}$$

Heat required to calcine TiO$_2$ from 100 C to 900 C

$$C_{p,TiO_2} @\ 100^\circ\mathrm{C} = 62.2\ \frac{J}{mol\ K}$$

$$C_{p,TiO_2} @\ 900^\circ\mathrm{C} = 76.2\ \frac{J}{mol\ K}$$

$$29.8\ kg * \frac{1\ mol}{80.0\ g} * \frac{1000\ g}{1\ kg} = 372.5\ mol$$

$$\Delta Q = (375.5\ mol)\left(\frac{76.2\frac{J}{mol\ K} + 62.2\frac{J}{mol\ K}}{2}\right) * (1173.15\ K - 373.15\ K)$$

$$\Delta Q = 2.079 * 10^{7} J = 20787\ kJ$$

Cooling time required after calcination

$$t = \frac{\rho c_p V}{hA}\ ln\ ln\ \left(\frac{T_f - T_\infty}{T_i - T_\infty}\right) = \frac{m c_p}{hA}\ ln\ ln\ \left(\frac{T_f - T_\infty}{T_i - T_\infty}\right)$$

$$A = \frac{\frac{\rho}{m}}{width} = \frac{\frac{4130\ kg/m^3}{29.38\ kg}}{0.001\ m} = 7.22\ m^2$$

$$t = \frac{(29.8\ kg)\left(848.6\frac{J}{kg\ K}\right)}{(10\frac{W}{m^2 K})(7.22\ m^2)}\ ln\ \left(\frac{900-25}{30-25}\right) = 1810\ s = 30.2\ min$$

A.8 Distillation Column

Distillation Column Size
Aspen Stages: 7 (5+ reboiler + condenser)
Packing Stages: 5
Feed Stage: 3
Diameter: 0.25 m
Bottom Holding Volume: 82.61L
Bottom Height: 1.05 m
Packing Height (HETP): 0.25 m

Height of Packing =Packing Height * Packing Stages
1.25 m = 0.25 * 5
Total Height = Top Height + Packing Height + Bottom Height
2.55 m = 0.25 + 1.25 + 1.052

Storage Tank
Daily Post-Washing Amount (From Aspen Simulation):
364 kg IPA → 463 L
1749 kg H_2O → 1749 L
Total Post-Washing Volume per Day: 2212 L
Tank Volume (17x the daily post-washing volume): 30966 L → 8181 Gal
Nominal Tank Size: 10000 Gal
No mixing is required (IPA is miscible in water)

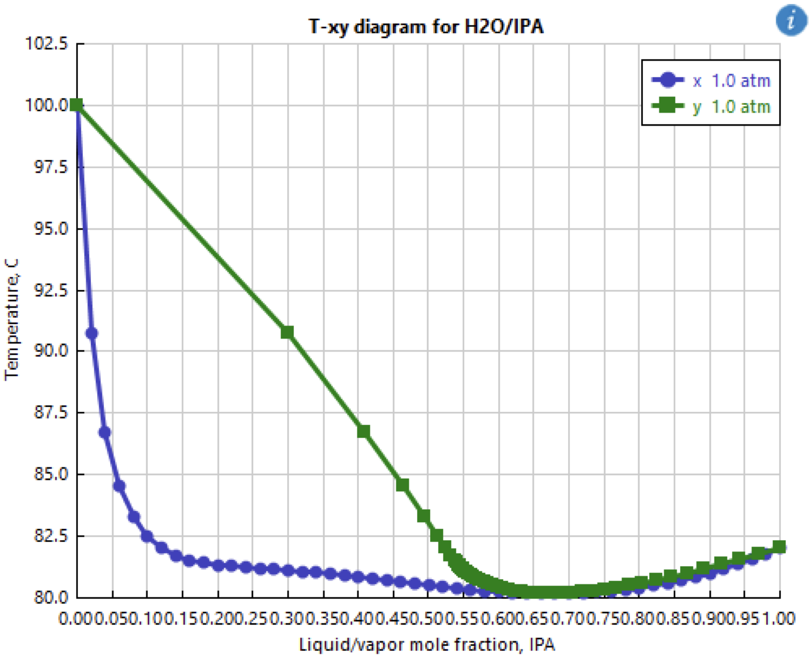


Figure 5: T-xy Diagram of IPA & Water

A.8.1 Reboiler

	Reboiler (0.0004 mol% IPA)	Steam
T_{in} (C)	100.01	165
T_{out} (C)	100.02	165

Stream	Heat Capacity (kJ/(kgK))	$\Delta H_{v,H}$ (kJ/kg)	Mass Flow (kg/hr)
Steam @ 7barg	-	2762	-
IPA Trace	4.184	-	137

From Aspen: Q = 50690 J/s
From PTW: U = 1200
From Figure 5: T_{sat} = 99 C

For Reboilers:

Phase Change dT_{lm}: $\Delta T_{lm} = \frac{(T_{H1}-T_{C1})-(T_{H2}-T_{C2})}{ln(\frac{T_{H1}-T_{C1}}{T_{H2}-T_{C2}})}$

$$Q = UA\Delta T_{lm}$$

$$50690\,W = 1200W/(m^2C) * A\,m^2 * 67.45C$$

Area of heat transfer: $A = 0.6m^2$

Mass of steam: $m = \frac{Q}{H_v} = \frac{50.7\ kW}{2762\ kJ/kg} = 1.8 \times 10^{-2} kg/s$

A.8.2 Condenser

	Condenser (77 mol% IPA)	Cooling Water
T_{in} (C)	82.86	30
T_{out} (C)	80.49	45

Stream	Heat Capacity (kJ/(kg K))	Mass Flow (kg/hr)
IPA Rich	3026	39.24
Cooling Water	4.184	1973

From Aspen: Q = -34392 J/s
From PTW: U = 1000 W/(m^2K)
T_{sat} = 80.35 C

For Condensers:

Phase Change dT_{lm}: $\Delta T_{lm} = \frac{(T_{H1}-T_{C1})-(T_{H2}-T_{C2})}{ln(\frac{T_{H1}-T_{C1}}{T_{H2}-T_{C2}})}$

$$Q = UA\Delta T_{lm}$$

$$-34392\, W = 1000W/(m^2C) * A\, m^2 * (-43.6\, C)$$

Area of heat transfer: $A = 0.79\, m^2$

Mass of cooling water: $m = \frac{Q}{C_p\Delta T} = \frac{34.39\, kW}{4.184kJ*(30-45)C} = 5.5 \times 10^{-1} kg/s$

A.8.3 IPA Stream for Sale

Since IPA is commonly sold with vol% labeling, our calculations related to this revenue stream will be in vol%.

Per day: 668 kg of 81 vol% IPA Produced

Volume: 807 L of 81 vol% IPA per day

$$M_1V_1 = M_2V_2$$

$$11.16 * 100 = 9.644 * V_2$$

$$V_2 = 115.72\, L$$

To make 70 vol% IPA, add 15.72 L of water for every 100 L of 81 vol% IPA.

Every Day: Add 127L of water to 807L of 81 vol% IPA to make 934L of 70 vol% IPA

Running 14 days in a cycle. One cycle is 29 days: 14 days running column, 15 days shut down.

Based on a 333-day operating year, there are 11.48 cycles in a year.

$$934L * 14 * 11.48 = 150075L \rightarrow 5074625\, fl.oz$$

A.9: Sunscreen Lotion Mixing

A.9.1 Aqueous mixing

Total volume needed for the tank

$$\frac{381\ L}{80\%\ working\ volume} = 476\ L = 126\ gallons \rightarrow 150\ gallons$$

With dimensions D_T = 97 cm and D_a = 32 cm

Assuming a tip speed of 5 m/s

$$\frac{5\frac{m}{s} \times 60\ sec}{\pi\ \times 0.32\ m} = 300\ RPM$$

Determining Reynolds number

$$\rho = \frac{357.2\ kg\ water + 29.8\ kg\ glycerin}{381\ L} = 1.02\frac{kg}{L} \rightarrow 1020\ \frac{kg}{m^3}$$

$$Re = \frac{(0.32\ m)^2(300/60\ RPS)(1020\frac{kg}{m^3})}{10^{-3}\ Pa\ s} = 5\ \times 10^5$$

Using a pitched blade impeller, N_p = 1.1

$$1.1 = \frac{P}{\left(\frac{300}{60}RPS\right)^3\ (1020\ \frac{kg}{m^3})(0.32\ m)^5} \rightarrow 470\ W$$

A.9.2 Oil phase mixing

Total volume needed for tank

$$\frac{116\ L}{80\%\ working\ volume} = 145\ L = 38\ gallons \rightarrow 38\ gallons$$

With dimensions D_T = 58 cm and D_a = 19 cm

Assuming a tip speed of 5 m/s

$$\frac{5\frac{m}{s} \times 60\ sec}{\pi\ \times 0.19\ m} = 500\ RPM$$

Determining Reynolds number

$$\rho(mixture) = \frac{11.9\ kg + 11.9\ kg + 5.95\ kg + 29.8\ kg + 29.8\ kg + 89.3\ kg + 29.8\ kg}{140.5\ L}$$
$$= 1.48\frac{kg}{L} \rightarrow 1484\ kg/m^3$$

$$Re = \frac{(0.19\ m)^2(500/60\ RPS)(1484\frac{kg}{m^3})}{10^{-3}\ Pa\ s} = 4\ \times 10^5$$

Using a pitched blade impeller, $N_p = 1.1$

$$1.1 = \frac{P}{\left(\frac{500}{60}RPS\right)^3\ (1484\ \frac{kg}{m^3})(0.19\ m)^5} \rightarrow 234\ W$$

A.9.3 Emulsion mixing

Total volume needed for the tank

$$\frac{497\ L}{80\%\ working\ volume} = 621\ L = 164\ gallons \rightarrow 200\ gallons$$

With dimensions D_T = 97 cm and D_a = 87 cm for the anchor impeller

Using a nominal 30 RPM mixing speed

Determining Reynolds number

Viscosity was found to be 0.0302 Pa s at 30 RPM using findings from Table 3 of Rasheed et al., 2012.

The combined density is 1200 kg/m^3

$$Re = \frac{(0.87\ m)^2(30/60\ RPS)(1200\frac{kg}{m^3})}{0.0302\ Pa\ s} = 15000$$

Using an anchor impeller, $N_p = 4$ (Furukawa, 2012))

$$4 = \frac{P}{\left(\frac{30}{60}RPS\right)^3\ (1200\ \frac{kg}{m^3})(0.87\ m)^5} \rightarrow 300\ W$$

A.9.4 Sunscreen Lotion Stream Table

Stream Name	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**	**S11**
kg/batch	119.1	11.9	29.8	11.9	29.8	202.5	357.6	29.8	387.4	6.0	595.9
Component Breakdown											
ZnO	89.3	-	-	-	-	89.3	-	-	-	-	89.3
H2O	-	-	-	-	-	-	357.6	-	357.6	-	357.6

TiO_2	29.8	-	-	-	-	29.8	-	-	-	-	29.8
Tridecyl Salicylate	-	11.9	-	-	-	11.9	-	-	-	-	11.9
Glyceryl Stearate	-	-	29.8	-	-	29.8	-	-	-	-	29.8
Dimethicone	-	-	-	11.9	-	11.9	-	-	-	-	11.9
Capric/Caprylic Triglyceride	-	-	-	-	29.8	29.8	-	-	-	-	29.8
Glycerin	-	-	-	-	-	-	-	29.8	29.8	-	29.8

A.10 Warming and Cooling Jackets

Jacket requirements:

Heating aqueous NaOH from 25°C to 90°C

$$\frac{18684\frac{mol}{batch} * 73.7\frac{J}{mol*K} * (363.15K - 298.15K)}{1800s} = 49.7kW\ required\ for\ heating$$

$$\frac{49.7kW}{2163.5\frac{kJ}{kg}} = 82.7\frac{kg}{h}\ of\ steam\ required\ for\ heating$$

$$\frac{49.7kW}{1500\frac{W}{m^2*K} * (406.15K - 363.15K)} = 0.77m^2\ of\ jacket\ area\ required\ for\ heating$$

Convective heat transfer in emulsion tank:

Correlation for a stirred tank using a paddle impeller

$$Nu = \frac{hD}{k} = .36Re^{.66}Pr^{.33}$$

$$Pr = \frac{C_p\mu}{k}$$

$$Q = hA\Delta T$$

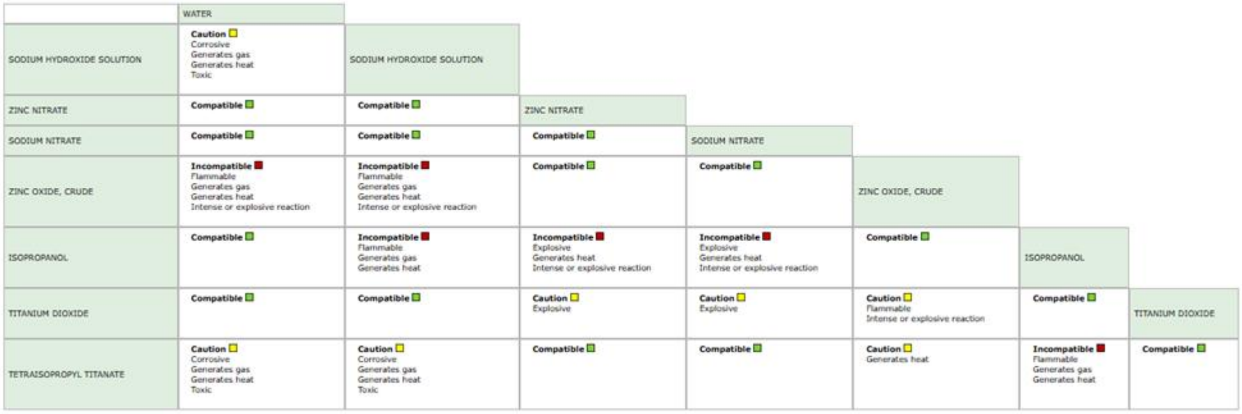
$$Nu = .36 * 15000^{.66} * 2.8^{.33} = 309$$

$$h = \frac{309 * 0.5918\frac{W}{mK}}{.97m} = 188.6\frac{W}{m^2K}$$

$$Q = 188.6\frac{W}{m^2K} * 2.3m^2 * (80C - 35C) = 19.5kW$$

A.11 Reactivity Matrix and ALOHA

CAMEO Chemicals Reactivity Matrix



	WATER	SODIUM HYDROXIDE SOLUTION	ZINC NITRATE	SODIUM NITRATE	ZINC OXIDE, CRUDE	ISOPROPANOL	TITANIUM DIOXIDE
SODIUM HYDROXIDE SOLUTION	**Caution** 🟨 Corrosive Generates gas Generates heat Toxic						
ZINC NITRATE	**Compatible** 🟩	**Compatible** 🟩					
SODIUM NITRATE	**Compatible** 🟩	**Compatible** 🟩	**Compatible** 🟩				
ZINC OXIDE, CRUDE	**Incompatible** 🟥 Flammable Generates gas Generates heat Intense or explosive reaction	**Incompatible** 🟥 Flammable Generates gas Generates heat Intense or explosive reaction	**Compatible** 🟩	**Compatible** 🟩			
ISOPROPANOL	**Compatible** 🟩	**Incompatible** 🟥 Flammable Generates gas Generates heat	**Incompatible** 🟥 Explosive Generates heat Intense or explosive reaction	**Incompatible** 🟥 Explosive Generates heat Intense or explosive reaction	**Compatible** 🟩		
TITANIUM DIOXIDE	**Compatible** 🟩	**Compatible** 🟩	**Caution** 🟨 Explosive	**Caution** 🟨 Explosive	**Caution** 🟨 Flammable Intense or explosive reaction	**Compatible** 🟩	
TETRAISOPROPYL TITANATE	**Caution** 🟨 Corrosive Generates gas Generates heat Toxic	**Caution** 🟨 Corrosive Generates gas Generates heat Toxic	**Compatible** 🟩	**Compatible** 🟩	**Caution** 🟨 Generates heat	**Incompatible** 🟥 Flammable Generates gas Generates heat	**Compatible** 🟩

ALOHA Parameters:

```
SITE DATA:
  Location: AUSTIN, TEXAS
  Building Air Exchanges Per Hour: 0.36 (sheltered single storied)
  Time: December 31, 2025  2359 hours CST (user specified)

CHEMICAL DATA:
  Chemical Name: ISOPROPANOL
  CAS Number: 67-63-0                    Molecular Weight: 60.10 g/mol
  PAC-1: 400 ppm      PAC-2: 2000 ppm     PAC-3: 12000 ppm
  IDLH: 2000 ppm      LEL: 20000 ppm      UEL: 127000 ppm
  Ambient Boiling Point: 179.1° F
  Vapor Pressure at Ambient Temperature: 0.023 atm
  Ambient Saturation Concentration: 23,179 ppm or 2.32%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 3 miles/hour from WNW at 3 meters
  Ground Roughness: open country          Cloud Cover: 0 tenths
  Air Temperature: 52° F                  Stability Class: F
  No Inversion Height                     Relative Humidity: 70%

SOURCE STRENGTH:
  Leak from hole in vertical cylindrical tank
  Flammable chemical escaping from tank (not burning)
  Tank Diameter: 8.5 feet                 Tank Length: 9.91 feet
  Tank Volume: 4207 gallons
  Tank contains liquid                    Internal Temperature: 52° F
  Chemical Mass in Tank: 10,115 kilograms
  Tank is 80% full
  Circular Opening Diameter: 3.6 inches
  Opening is 0 feet from tank bottom
  Ground Type: Concrete
  Ground Temperature: equal to ambient
  Max Puddle Diameter: Unknown
  Release Duration: ALOHA limited the duration to 1 hour
  Max Average Sustained Release Rate: 49.3 pounds/min
     (averaged over a minute or more)
  Total Amount Released: 2,194 pounds
  Note: The chemical escaped as a liquid and formed an evaporating puddle.
  The puddle spread to a diameter of 61 yards.
```

Appendix B: Economic Calculations

B.1 Capital Investment

Capital costs were determined from online purchase prices of various equipment types or using tables from Turton, 2012, and PTW, 2003. Equipment prices with tables were updated to current pricing using the following formula. The tables for Turton use a CEPCI from 2001 and PTW in 2002. They are 397 and 396, respectively.

$$C_{2025} = C_{200X}\left(\frac{CEPCI_{2025}}{CEPCI_{200X}}\right)$$

Storage Tank Capital Cost

All storage tanks were sized by the volume requirement of 30 days for raw materials. The nearest nominal tank size was chosen considering providing adequate extra capacity in case of overfilling or schedule delays.

Table B.1.1 Storage Tank Costs and Sources

Storage Tank	Purpose	Size (Gal)	Quantity	Cost	Note
ST-1	ZNH	-	1	-	Powder will be stored in the original shipping package
ST-2	NaOH	2500	1	$ 2,770.00	NTO Tank
ST-3	TTIP	1000	1	$ 8,928.00	Glacier Tank
ST-4	Washing Waste for Distillation	2500	1	$ 2,770.00	NTO Tank
ST-5	IPA for Washing	5000	1	$ 9,530.00	NTO Tank
ST-6	Tridecyl Salicate	120	1	$ 487.00	Performance Supply
ST-7	Glyceryl Stearate	330	1	$ 1,452.00	
ST-8	Capric/Caprylic Triglyceride	330	1	$ 1,452.00	
ST-9	Glycerin	240	1	$ 1,039.00	
ST-10	Styrene Acrylate Co-Polymer	70	1	$ 316.00	
ST-11	Dimethicone	70	1	$ 361.00	

Pump Capital Cost & Power Consumption

Our centrifugal pumps were priced based on their shaft power, resulting in an average cost of \$253 per pump. This aligns with the range that Pump World has priced for their low-flow rate centrifugal pumps. With 1 additional spare for each pump, the total cost for our pumps is \$11,123.43. The power consumption of each pump was from Turton’s Table 11.9 Heuristics for Pumps. Using Turton’s Figure A.3, which relates pump power and pricing, our pump was priced accordingly and then scaled using CEPCI. The ratio, adjusted to 2025 CEPCI, was \$2317.38/kW. The efficiency of all our pumps was 70%.

$$P = \frac{1.67 * dP * V}{\varepsilon}$$

P - Power (kW)

dP - pressure differential (bar)

V - volumetric flow rate (m^3/min)

ε - pump efficiency

Table B.1.2 Pump Cost & Parameters

Pump	**Description**	**V (L/min)**	Cost	**Power (kW)**	**dP (bar)**
P1	Water for $Zn(NO_3)_2$ 6 H_2O preparation	143	$802	0.346	1.01
P2	NaOH Feed	15	$109	0.047	1.28
P3	$Zn(NO_3)_2$ $6H_2O$ Feed to Batch	122	$776	0.335	1.15
P4	Batch effluent	139	$1,339	0.578	1.62
P5	Washing Water (ZnO)	58	$327	0.141	1.01
P6	Resuspended ZnO to C-1	58	$359	0.155	1.11
P7	Water feed (TiO_2 reactor)	1	$5	0.002	1.65
P8	TTIP feed	0.4	$2	0.001	1.14
P9	TiO_2 to MT-3	1	$7	0.003	1.56
P10	MT-3 to centrifuge	53	$320	0.138	1.09
P11	Washing Water (TiO_2)	47	$260	0.112	1.01
P12	Resuspended TiO_2 to C-1	42	$255	0.11	1.09
P13	ST-4 to Distillation	48	$324	0.14	1.22
P14	Distillation Reflux	1	$14	0.006	1.76
P15	ST-5 to wash	22	$125	0.054	1.01
P16	ST-6 to oil mixing	1	$5	0.002	1.13
P17	ST-8 to oil mixing	2	$14	0.006	1.11
P18	ST-9 to aqueous mixing	2	$9	0.004	1.14
P19	Water to aqueous mixing	26	$144	0.062	1.01
P20	Oil Mixing Effluent	5	$30	0.013	1.06
P21	Aqueous Mixing Effluent	26	$153	0.066	1.06
P22	Emulsion Mixing Effluent	31	$183	0.079	1.07
Number of Spares					22

Pump	**Description**	**V (L/min)**	Cost	**Power (kW)**	**dP (bar)**
Total Cost		$ 11,123			
Cost Per Pump		$ 253			

Mixing Tank Capital Cost

Mixing tanks with their impellers and drivers were priced using current online vendors and PTW figures 12-42 and 12-52. The cost is scaled from CEPCI 2002 to 2025. In Table B.1.2, all impeller costs include the driver.

Table B.1.3 Mixing Tank Cost and Source

Mixing Tank	**Description**	**Specification**	**Cost**	**Pricing Source**
MT-1	ZNH preparation	1000 gal tank	$49,000	LabX
		0.5 m pitch-blade impeller		
MT-2	ZnO Washing	1000 gal tank	$22,222	PTW
		0.61 m Rushton impeller	$17,128	PTW
MT-3	TiO_2 Slurry	200 gal tank	$5,469	INDCO
		0.32 m Rushton impeller	$20,151	PTW
MT-4	TiO_2 Washing	200 gal tank	$5,469	INDCO
		0.32 m Rushton impeller	$20,151	PTW
MT-6	Oil Mixer	38 gal tank	$3,553	INDCO
		0.19 m pitched-blade impeller	$9,824	PTW
MT-5	Aqueous Mixer	150 gal tank	$5,325	INDCO
		0.32 m pitched-blade impeller	$5,038	PTW
MT-7	Emulsion Mixer	200 gal tank	$5,469	INDCO
		0.032 m high shear impeller	$21,176	ROSS

		0.87 m anchor impeller	$10,811	LAB TECH SALES

Stirred Reactor Capital Cost

The costs for our stirred and jacketed reactors are from PTW Figure 13-15. All our reactors are made of stainless steel and priced using CEPCI.

B.1.4 Stirred Reactor Cost

Stirred Reactor	Description	Specification	Cost
SR-1	ZnO Reactor	1000 gal	$ 161,616
SR-2	TiO_2 Reactor	90 gal	$ 23,232

Rotary Dryer/Kiln Capital Cost

Rotary dryers and the calciner were priced using the surface area and Turton 2012's Figure A.12.

B.1.5 Dryer Cost

Dryer	Description	Surface Area (m^2)	Cost
D-1	ZnO	84.8	$ 529,877
D-2	TiO_2	33.9	$ 249,555
D-3	Calciner	6.28	$ 50,645

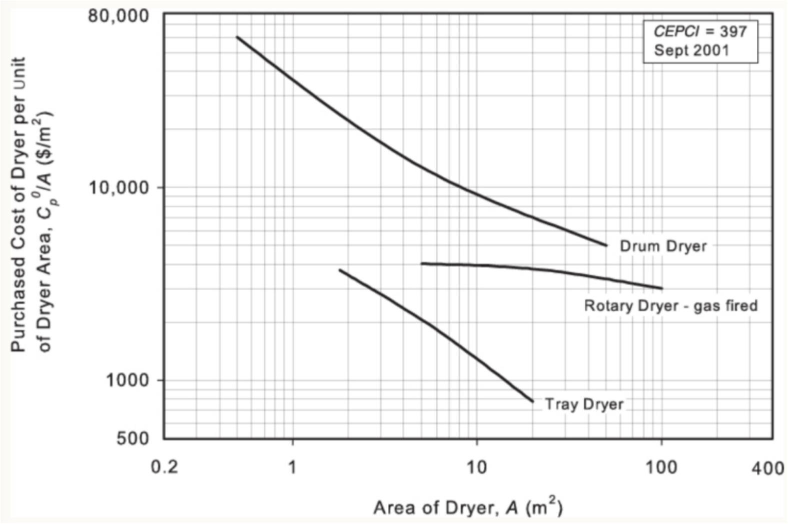


Figure B.1: Purchased Costs For Dryers (Turton, 2012)

Heat Exchanger Capital Cost

Heat exchanger cost was determined using Figure A.5 from Turton. The CEPCI in 2002 was 396. And our CEPCI used for 2025 is 800.

Table B.1.6 Heat Exchanger Cost

Heat Exchanger	Description	Area m2	Quantity	Cost
H1	Condenser	0.79	1	$ 2,222.22
H2	Reboiler	0.63	1	$ 2,424.24

Centrifuge Capital Cost

The cost of our centrifugal separators is $23,275 for ZnO and $22,972 for TiO_2. This was determined with the centrifuge diameter of 1m each and Figure A.9 in Turton 2012. A sample calculation for the ZnO centrifuge is provided below.

$$C_{2025} = C_{2001}(\frac{CEPCI_{2025}}{CEPCI_{2001}}) = \$11600 * \frac{800}{397} = \$23,375.31$$

Distillation Column Capital Cost

The cost for our vertical column made of 316 stainless steel (2.6m in height) was determined in Figure 15-11 in Peters et al., 2003 to be \$30,226.70. Referencing PTW Figure 15-14, the purchase cost for 0.3 m^3 of packing is \$303.03.

Powder Blender & Finishing Mill Capital Cost

The powder blender was priced using Figure A.8 from Turton 2012. The cost of the blender per unit of volume was \$10,700 per m^3. Using a CEPCI of 800 to their reference CEPCI of 397, the powder blender cost \$1509. The finishing mill was sourced from Sweco to be \$3000.

Table B.1.7 Equipment Cost

Equipment Type	**Equipment Name**	**Cost per unit**	**Quantity**	**Total Cost**
Pumps	P1, P2, ...P22	$253	44	$11,123
Mixing Tank	MT-1	$49,000	1	$49,000
Mixing Tank	MT-2	$22,222	1	$22,222
Mixing Tank	MT-3, MT-4, MT-7	$20,151	3	$60,453
Mixing Tank	MT-6	$9,824	1	$9,824
Mixing Tank	MT-5	$5,038	1	$5,038
20" Pitch Blade Impeller	I-1	(Included in Tank Price)	1	$0
24" Pitch Blade Impeller	I-2	$17,128	1	$17,128
13" Rushton Impeller	I-3, I-4	$20,151	1	$20,151
8" Pitch Blade Impeller	I-5	$9,824	1	$9,824
13" Pitch Blade Impeller	I-6	$5,038	1	$5,038

Equipment Type	**Equipment Name**	**Cost per unit**	**Quantity**	**Total Cost**
High Shear Impeller	I-7	$21,176	1	$21,176
Anchor Impeller	I-8	$10,811	1	$10,811
Stirred Reactor	SR-1	$161,616	1	$161,616
Stirred Reactor	SR-2	$23,232	1	$23,232
Heat Exchanger	H-1	$2,222	1	$2,222
Heat Exchanger	H-2	$2,424	1	$2,424
Centrifuge	C-1	$23,375	1	$23,375
Centrifuge	C-2	$22,972	1	$22,972
Rotary Dryer	D-1	$529,877	1	$529,877
Rotary Dryer	D-2	$249,555	1	$249,555
Rotary Kiln	D-3	$50,645	1	$50,645
Distillation Column	DC-1	$30,227	1	$30,227
Column Packing	DC-2	$303	1	$303
Storage Tank	ST-2, ST-4	$2,770	2	$5,540
Storage Tank	ST-3	$8,928	1	$8,928
Storage Tank	ST-5	$9,530	1	$9,530
Storage Tank	ST-6	$487	1	$487
Storage Tank	ST-7, ST-8	$1,452	2	$2,904
Storage Tank	ST-9	$1,039	1	$1,039
Storage Tank	ST-10, ST-11	$316	2	$632
Powder Blender	PB-1	$1,509	1	$1,509
Finishing Mill	B-1	$3,000	1	$3,000
Intermediate Plastic Drums	DR-1, DR-2, ... DR-6	$47	6	$282
Total				$1,372,089

B.2 Operating Costs

B.2.1 Raw Materials

B.2.1-1 Raw Material Costs

Material	**Cost Per MT**	**MT per year**	**Total Cost**
Zinc Nitrate Hexahydrate	28760	121	$3,475,00
TTIP	36353	22	$803,000
Dimethicone	14815	4	$59,000
Tridecyl Salicylate	100	4	$400
Styrene/Acrylate Copolymer	7800	2	$15,500
Glyceryl Stearate	3240	10	$32,000
Capric Triglyceride	12668	10	$126,000
Glycerin	1945	10	$19,000
	Cost Per Gal	**Gal per Year**	
Sodium Hydroxide	6	27042	$168,000
50% IPA (Initiate Process)	14	149	$2,000
Total Cost of Raw Materials			$4,700,000

B.2.2 Utilities

Table B.2.2-1 Utility Costs

Equipment	**Electricity Cost ($/year)**	**Steam Cost ($/year)**	**Cooling Water Cost ($/year)**
	\$0.12 / kWh	\$4.40 / 1000 kg	\$0.07 / m^3
Pumps	24.55	-	-
Condenser	-	-	533.00
Reboiler	-	1,099.00	-
Jackets	-	223.00	31,300.00
Mixing Tanks	68,900.00	-	-
Dryers	600.00	-	-
Milling	1,490.00	-	-
Powder Blending	10.00	-	-
Centrifuging	2,770.00	-	-
Calciner	416.00	-	-
Total Costs	**74,210.00**	**1,322.00**	**31,833.00**

B.2.2-2 Process Water Costs

	Process Water Cost ($/year)
Process	$1.10 / m^3
MT-1	738.00
MT-2	2,684.00
MT-3	53.33
MT-4	573.00
MT-5	131.00
IPA Product	25.95
Total Costs	**4,205.00**

B.2.3 Waste Disposal Costs

Table B.2.3-1 Wastewater disposal costs

Waste Stream	**Gallons/day**	**Gallons/year**
ZnO Wash	867	288800
Bottoms Distillation Product	3383	1126623
Total	4250	14154232

$11.30 per 1000 gallons → $12,600 per year

Table B.2.3-2 ZnO Wash Stream Breakdown

	kg/day
Water	12807.0
Sodium Nitrate	186.6
Zinc Nitrate	36.2
Sodium Hydroxide	9.8

$0.53 per 1000 kg → $230,136 per year

Total Waste Cost: $246,896 per year

B.2.4 Labor

Table B.2.4-1 Worker requirements based on Peters et al. 2003

Type of Equipment	**Worker/unit/shift**	**No. Units**	**Worker/shift**
Blowers and Compressors	0.100	0	0
Centrifugal separator	0.250	2	0.5
Crystallizer	0.160	0	0
Dryer, rotary	0.500	3	1.5
Dryer, spray	1.000	0	0
Dryer, tray	0.500	0	0
Evaporator	0.250	0	0
Filter, vacuum	0.125	0	0
Filter, plate, and frame	1.000	0	0
Filter, rotary, and belt	0.100	0	0
Heat exchange	0.100	2	0.2
Process vessels, towers	0.200	9	1.8
Reactor, batch	1.000	1	1
Reactor, continuous	0.500	1	0.5
Total	-	-	5.5

5.5 workers/shift → 6 workers/shift

6 * 4.5 = 27 operators required

Operator costs per year:

6 workers per hour * 8000 working hours * $50.30 = $2,414,400 per year

Supervisor costs:

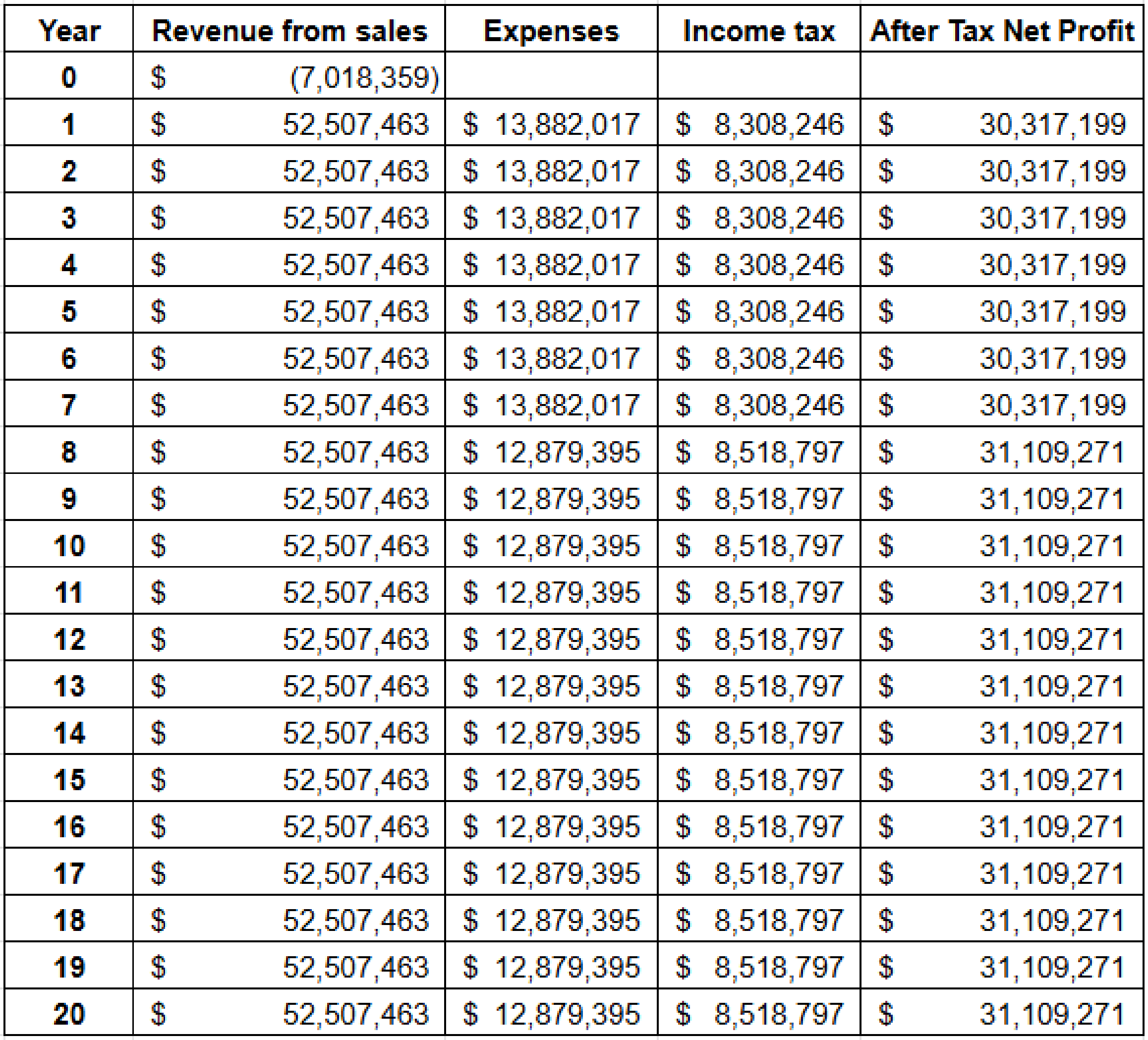
0.15 * operator costs = 0.15 * 2,414,400 = $362,160 per year

Total operating costs, including benefits

1.5 * (operator costs + supervisor costs) = 1.5 * (2,414,400 + 362,160) = $ 4,164,840 per year

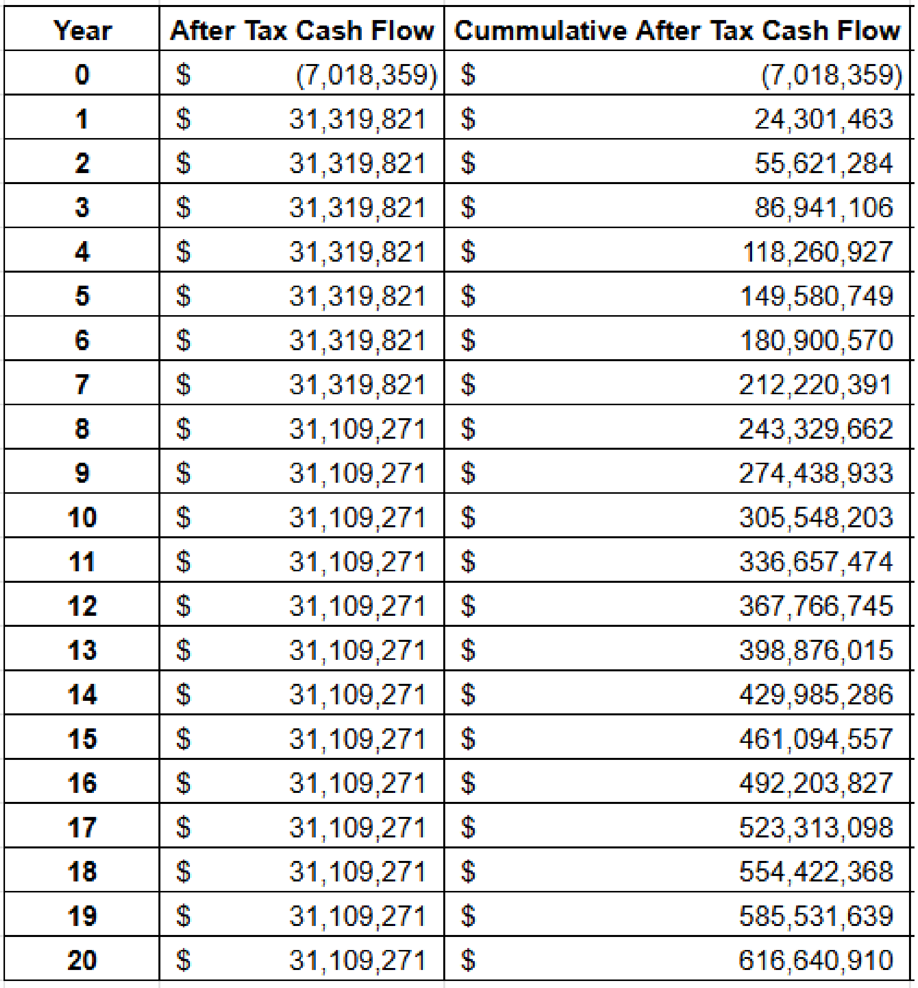
B.3 Economic Analysis

Table B.3-1 Net Profit of Total Production



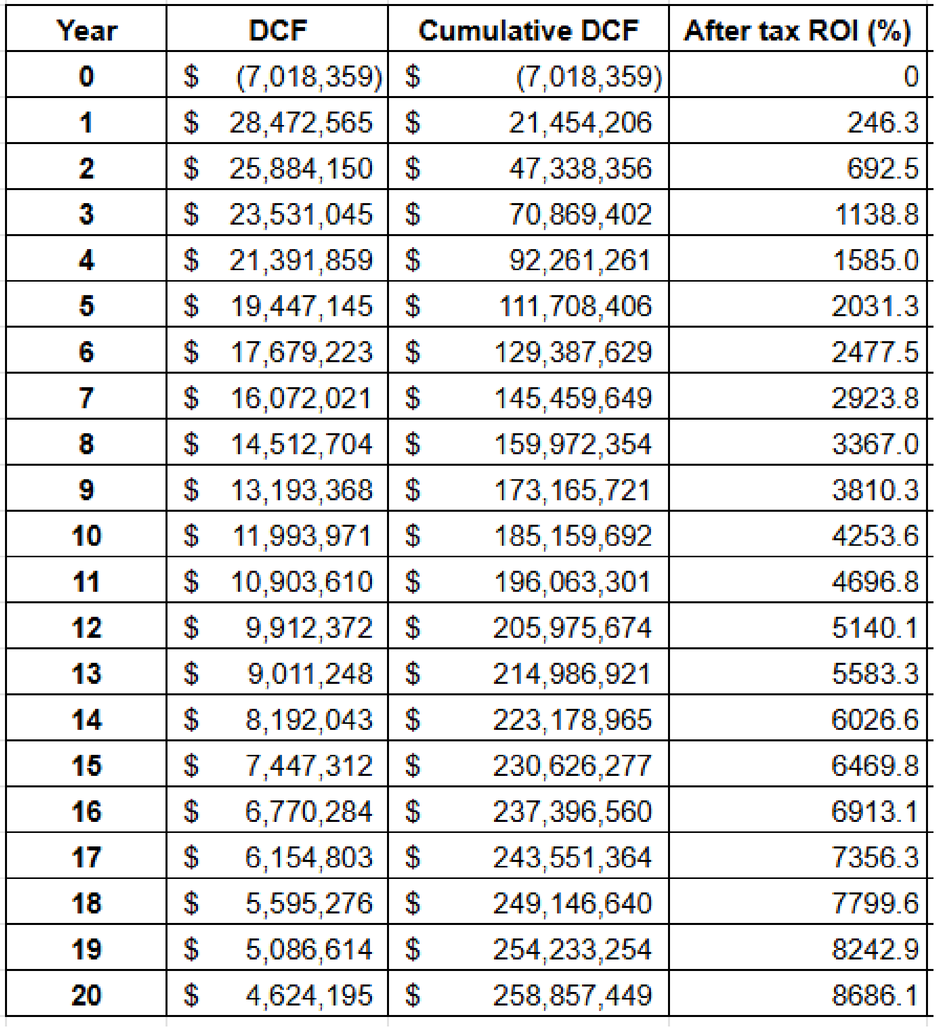
Year	Revenue from sales	Expenses	Income tax	After Tax Net Profit
0	$ (7,018,359)			
1	$ 52,507,463	$ 13,882,017	$ 8,308,246	$ 30,317,199
2	$ 52,507,463	$ 13,882,017	$ 8,308,246	$ 30,317,199
3	$ 52,507,463	$ 13,882,017	$ 8,308,246	$ 30,317,199
4	$ 52,507,463	$ 13,882,017	$ 8,308,246	$ 30,317,199
5	$ 52,507,463	$ 13,882,017	$ 8,308,246	$ 30,317,199
6	$ 52,507,463	$ 13,882,017	$ 8,308,246	$ 30,317,199
7	$ 52,507,463	$ 13,882,017	$ 8,308,246	$ 30,317,199
8	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
9	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
10	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
11	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
12	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
13	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
14	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
15	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
16	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
17	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
18	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
19	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271
20	$ 52,507,463	$ 12,879,395	$ 8,518,797	$ 31,109,271

Table B.3-2 After-Tax Cash Flow of Total Production



Year	After Tax Cash Flow	Cummulative After Tax Cash Flow
0	$ (7,018,359)	$ (7,018,359)
1	$ 31,319,821	$ 24,301,463
2	$ 31,319,821	$ 55,621,284
3	$ 31,319,821	$ 86,941,106
4	$ 31,319,821	$ 118,260,927
5	$ 31,319,821	$ 149,580,749
6	$ 31,319,821	$ 180,900,570
7	$ 31,319,821	$ 212,220,391
8	$ 31,109,271	$ 243,329,662
9	$ 31,109,271	$ 274,438,933
10	$ 31,109,271	$ 305,548,203
11	$ 31,109,271	$ 336,657,474
12	$ 31,109,271	$ 367,766,745
13	$ 31,109,271	$ 398,876,015
14	$ 31,109,271	$ 429,985,286
15	$ 31,109,271	$ 461,094,557
16	$ 31,109,271	$ 492,203,827
17	$ 31,109,271	$ 523,313,098
18	$ 31,109,271	$ 554,422,368
19	$ 31,109,271	$ 585,531,639
20	$ 31,109,271	$ 616,640,910

Table B.3-3 DCF Analysis and After-tax ROI of Total Production



Year	DCF	Cumulative DCF	After tax ROI (%)
0	$ (7,018,359)	$ (7,018,359)	0
1	$ 28,472,565	$ 21,454,206	246.3
2	$ 25,884,150	$ 47,338,356	692.5
3	$ 23,531,045	$ 70,869,402	1138.8
4	$ 21,391,859	$ 92,261,261	1585.0
5	$ 19,447,145	$ 111,708,406	2031.3
6	$ 17,679,223	$ 129,387,629	2477.5
7	$ 16,072,021	$ 145,459,649	2923.8
8	$ 14,512,704	$ 159,972,354	3367.0
9	$ 13,193,368	$ 173,165,721	3810.3
10	$ 11,993,971	$ 185,159,692	4253.6
11	$ 10,903,610	$ 196,063,301	4696.8
12	$ 9,912,372	$ 205,975,674	5140.1
13	$ 9,011,248	$ 214,986,921	5583.3
14	$ 8,192,043	$ 223,178,965	6026.6
15	$ 7,447,312	$ 230,626,277	6469.8
16	$ 6,770,284	$ 237,396,560	6913.1
17	$ 6,154,803	$ 243,551,364	7356.3
18	$ 5,595,276	$ 249,146,640	7799.6
19	$ 5,086,614	$ 254,233,254	8242.9
20	$ 4,624,195	$ 258,857,449	8686.1

$$Total\ Operating\ Cost\ = Raw\ Materials + Waste\ Management + Utilities + Labor$$

$$Straight - line\ Depreciation = \frac{Capital\ Cost}{7\ years}$$

$$Expenses = Total\ Operating\ Cost + Depreciation$$

$$Income\ Tax = (Revenue - Expenses) * Tax\ Rate$$

$$Federal\ Income\ Tax = 21\% \quad Texas\ Franchise\ Tax = 0.375\%$$

$$Tax\ Rate = Federal\ Income\ Tax * (Revenue - Expenses) + Texas\ Franchise\ Tax * (Revenue)$$

$$After\ Tax\ Net\ Profit = Revenue - Expenses - Income\ Tax$$

$$After\ Tax\ Cash\ Flow = After\ Tax\ Net\ Profit + Depreciation$$

$$Discounted\ Cash\ Flow = \frac{After\ Tax\ Cash\ Flow}{(1 + Discount\ Rate)^{year}}$$

$$Discount\ Rate = 10\%$$

$$After\ Tax\ ROI = \frac{Cumulative\ After\ Tax\ Cash\ Flow - Capital\ Cost}{Capital\ Cost} * 100\%$$