

AICHE Design Competition 2017
Nylon-6,6 Production Facility

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Abstract

Nylon-6,6 is a synthetic polymer that is manufactured from Adipic Acid and Hexamethylenediamine (HMDA). This report outlines the process design and economic analysis for the construction of a grassroots plant for the production of 85 million lbs/year of Nylon-6,6. For this design, a batch process was selected. Four reactors are utilized, and four complete cycles of each reactor are run per day. The economic analysis was performed over a span of fifteen years, assuming ten year MACRS depreciation on capital costs. A minimum rate of return of 15% was assumed. The net present value of the Nylon-6,6 production plant is \$69,300,000 at 100% capacity. The discounted cash flow rate of return is 113%.

The process has been determined profitable and feasible after a technical, safety, and economic evaluation. It is recommended that this project move into the next stage of detailed design utilizing the process design described in this report.

Introduction

Nylon-6,6 is a manufactured polymer that is produced in the reaction between Adipic Acid and HMDA. Its chemical formula is $(C_{12}H_{22}N_2O_2)_n$. Nylon-6,6 is a common material used to make carpet and other floor coverings, upholstery, conveyor belts and tires, clothing, coated fabrics, toothbrushes, hangers, and packaging. Nylon, compared to others polymers, is a preferred material because of its high tensile strength, durability, and melting point.³ Nylon-6,6 is named because of the amount of carbons that the amine and acid group contribute to the molecule, as seen in the reaction below:

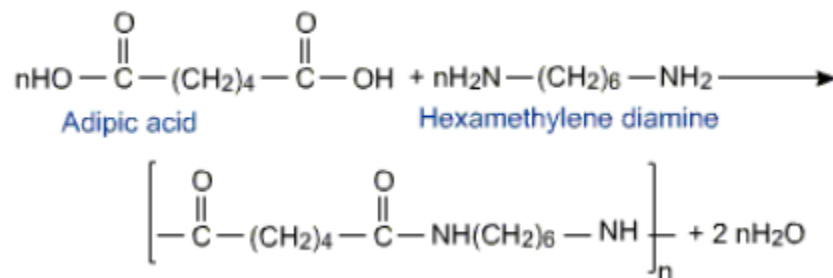


Figure 1: Reaction to form Nylon-6,6

Nylon-6,6 has advantages over other types of nylon such as abrasion resistance, low shrinkage at high temperatures, and a less open structure, which makes Nylon-6,6 better for dyeing and more resistant to change in color from exposure to UV light.³

In this manufacturing process, Adipic Acid and HMDA react in a polymerization reaction to form Nylon-6,6 and water, as shown above in Figure 1. The process begins when Adipic Acid and HMDA are mixed in stoichiometric amounts and are combined with water in a mixer. The mixture is heated to approximately 266 °F, which is the

temperature required to dissolve the Adipic Acid and HMDA in water, and the solution becomes a molten salt. Before this solution is transferred to the polymerization reactor, the reactor is purged with nitrogen to eliminate the presence of any oxygen, which could lead to degradation of the Nylon-6,6. After the purge is complete, the solution is transferred to a jacketed batch polymerization reactor and the dissolved products react to form Nylon-6,6 and water. The reactor temperature is raised to approximately 478°F while the water product and the water used to dissolve the reactants evaporates off of the reactor and is vented to atmosphere. As more steam is vented, the polymerization reaction is driven forward to produce more Nylon-6,6. After the water content has been reduced in the reactor to 0.2% by mass, the product nylon in a molten state is transferred to an extruder where it is extruded and cut into chips at a final product amount of approximately 259,000 lbs/day.

Though there has been an industry shift in recent years to the use of a continuous process for producing polymers, a batch process has been evaluated to be more easily controlled and to have greater scaling capabilities if demand decreases. In this design, four cycles of a complete batch are produced per day in order to minimize the size of the equipment required. During one cycle, four mixers and four polymerization reactors are used, further reducing the size of each piece of equipment needed. Stainless steel is used for each mixer and reactor due to the corrosive nature of the reactants. A simple schematic of the process is shown in Figure 2, below.

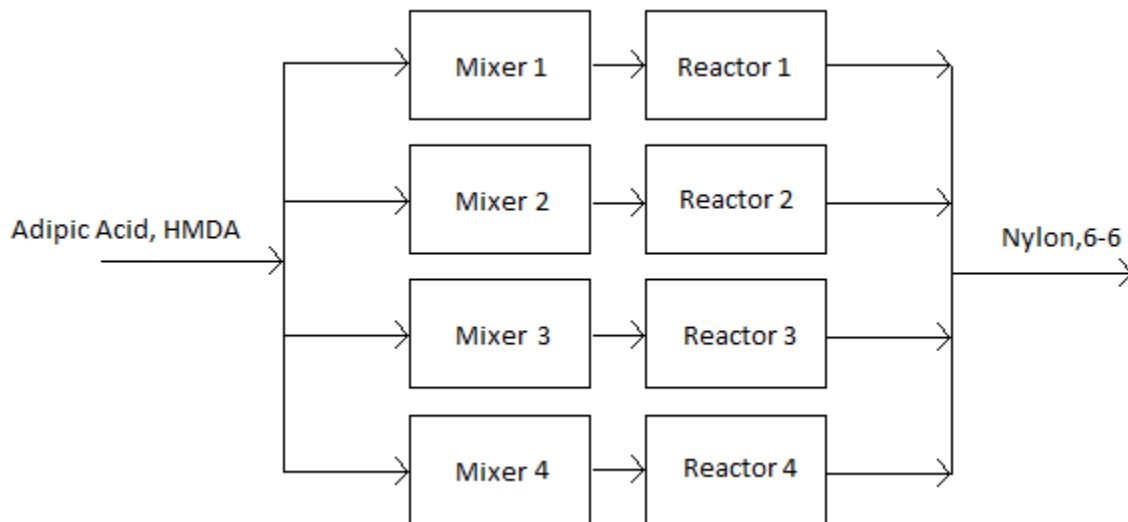


Figure 2: Block Flow Diagram of Mixer/Reactor Pairs

Electric heating is used in the mixer and the polymerization reactor rather than steam due to local utility costs. Heat and material integration designs have been evaluated and not deemed profitable for the process. Steam produced in the polymerization reactor could be used to preheat the water used to dissolve the reactants, but the timing of the steam vent to atmosphere does not correspond with the timing of the water feed to the mixer. Condensing, treating, and recycling steam to the feed water tank was evaluated

as a form of material integration. Material integration was rejected because the operating cost of the heat exchanger far surpassed the cost of purchasing water. A recycle stream for the HMDA and Adipic Acid was not determined necessary during the preliminary design process due to high conversion of reactants, though further investigation is recommended in later stages of the design process.

Management has determined the plant location to be Calvert City, Kentucky. This plant will have the capability to produce 85 million pounds of Nylon-6,6 annually. Because it is a batch process, production can be scaled down to any desired amount by operating less frequently on the installed equipment. Calvert City is located on the Tennessee River and the Paducah and Louisville railways. This makes Calvert City an optimal location for transportation into and out of the plant. It is located in a central geographic region and there are no notable barriers to transportation in the area. The current purchase price of the reactants and sale price of the Nylon-6,6 product, which can be seen below in Table 1, make this process very valuable at this time, and thus construction in 2018 and startup in mid-2019 would be optimal.

Table 1: Commodity Prices

Material	Price Per Pound
Adipic Acid	\$0.61
HMDA	\$1.12
Nylon-6,6	\$1.36

The assumed minimum rate of return is 15%. This grassroots project will be evaluated over a 15 year span, assuming ten year MACRS depreciation of capital investments. The design will be analyzed for 100% capacity operation as well as 67% capacity operation.

A thorough hazard identification has been completed and a hazard mitigation plan has been produced. A complete discussion of the hazards associated with each material and operation in the process begins on page 34 of this document. Safety Data Sheets are also included on pages 81 through 96 in the Appendix. The process involves the use of materials that pose significant potential to be hazardous to both plant personnel and the environment. Care has been taken to minimize the risk posed by the use of materials and severe operating conditions. The main safety concerns in this process involve high temperatures and combustion. If molten Nylon-6,6 comes in contact with skin or clothing, severe burns will occur. HMDA and Adipic Acid are both toxic and can cause burns, blisters, and severe irritation if not properly contained. Wastewater treatment is also critical in the process, as HMDA and Adipic Acid are both highly toxic to aquatic life.

The process, equipment, costing, and safety information for the preliminary design is given in the remainder of this document.

Process Flow Diagram and Material Balances

The process flow diagram (PFD) for the process can be seen on pages 10 and 11 of this document. The key in the bottom right corner gives insight to labeling information. A detailed controls scheme for the mixers and polymerization reactors is give on page 12. A stream summary table for each process stream can be found on page 13. A detailed description of the process will be given in the subsequent sections of this document.

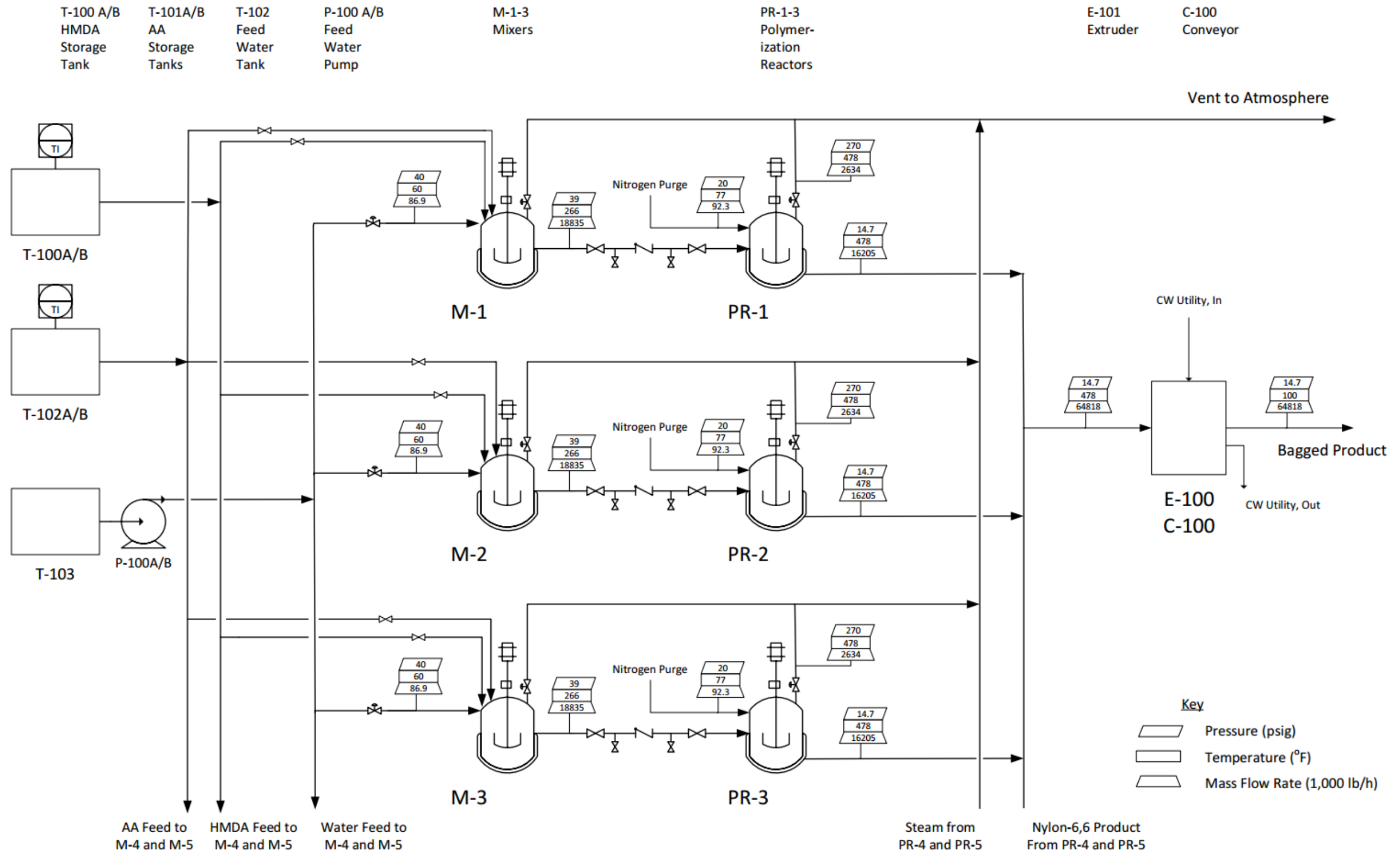


Figure 3: Process Flow Diagram 1 of 2

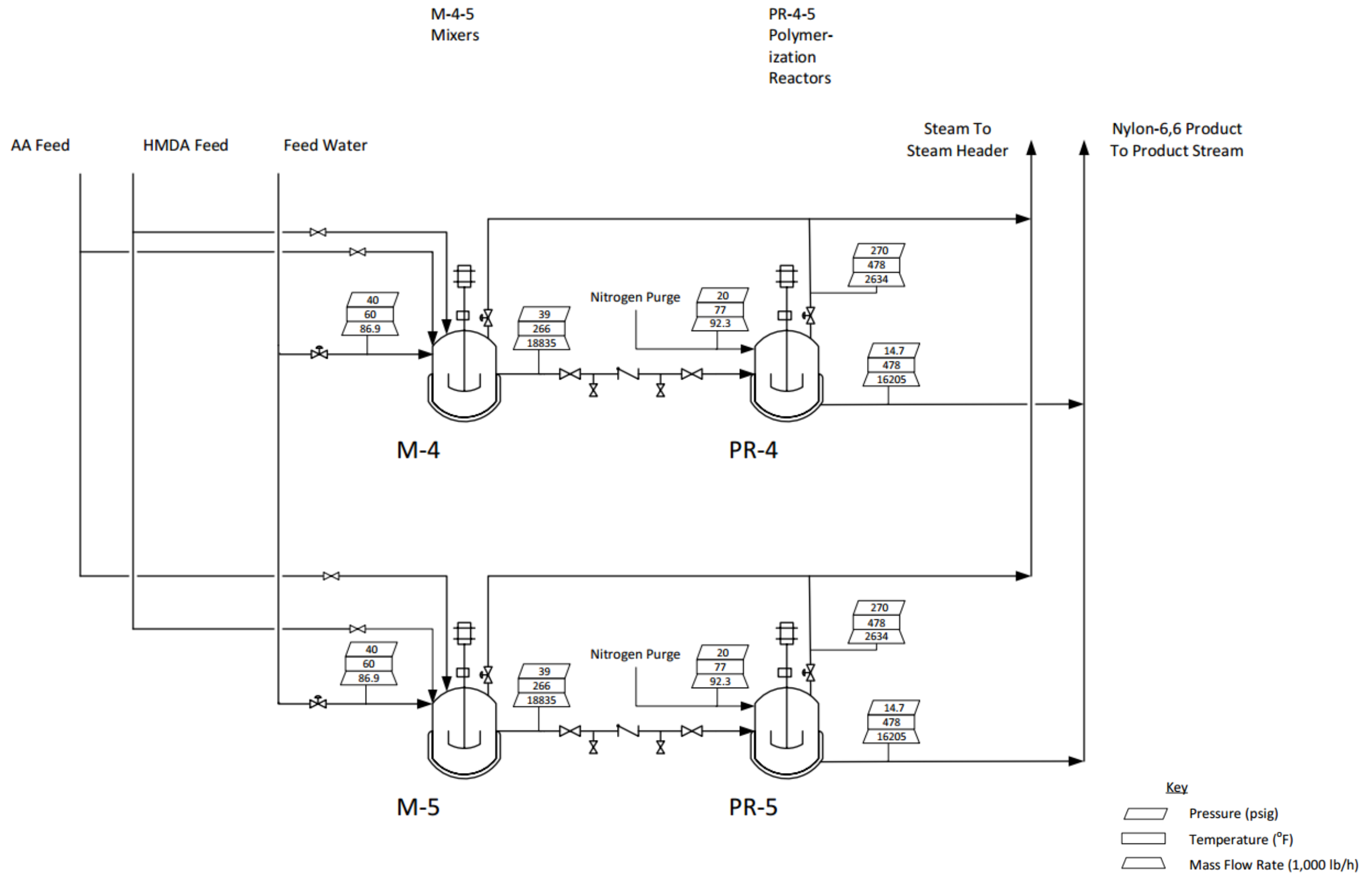


Figure 4: Process Flow Diagram 2 of 2

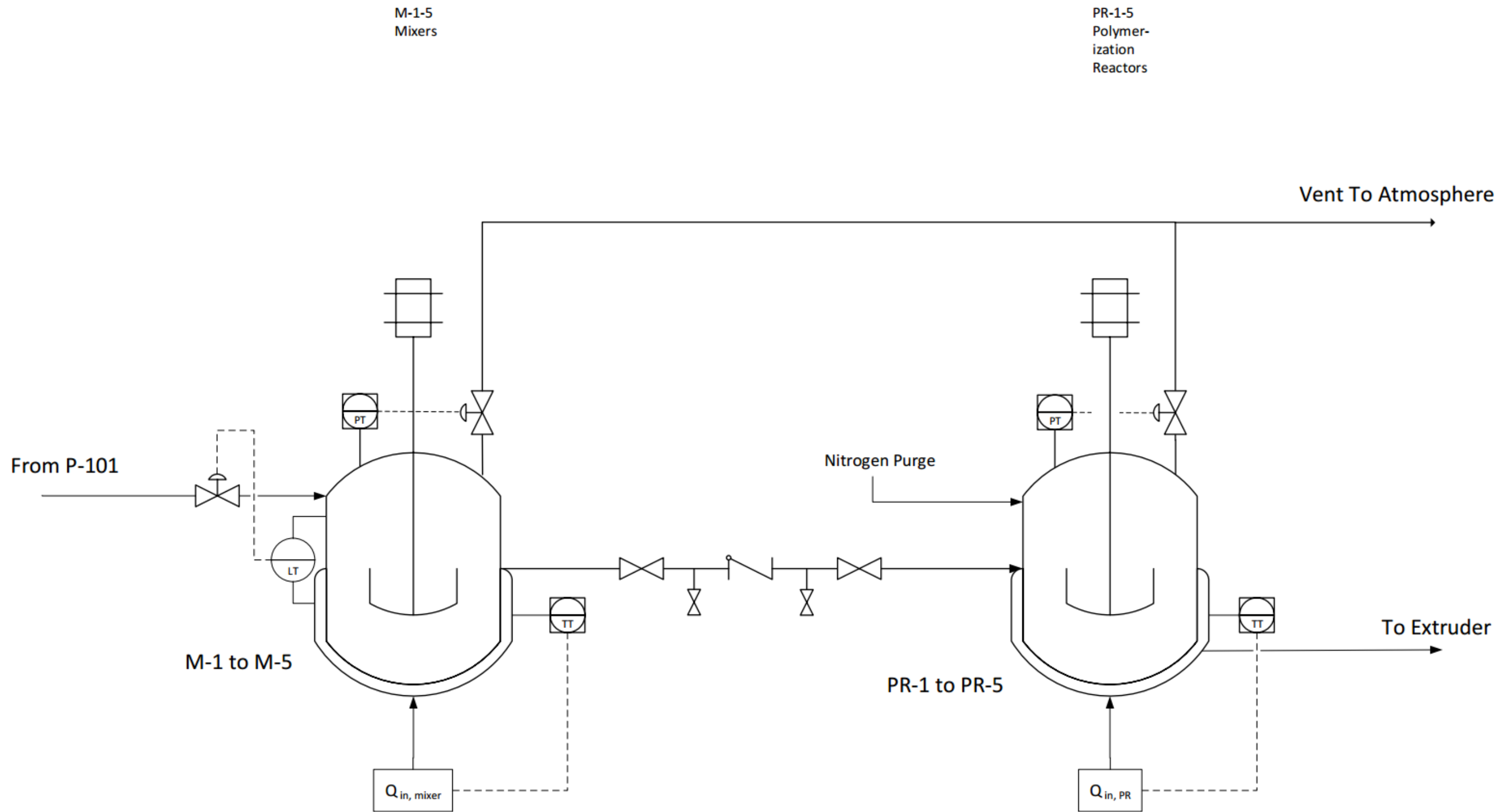


Figure 5: Controls Scheme for Reactors and Mixers

Stream Number	1	2	3	4	5	6	7	8	9	10
Stream Label	Adipic Acid Feed	HMDA Feed	Water Feed to Pump	Water Feed to Mixer	Adipic Acid/HMDA Solution	Feed to Reactor	Nitrogen Purge	Steam	N66 Feed to Extruder	Product Stream
Phase	Solid	Solid	Liquid	Liquid	Liquid	Liquid	Vapor	Vapor	Liquid/Molten	Solid
Pressure, psi	14.7	14.7	14.7	40	39	39	20	270 (max)	14.7	14.7
Temperature, °F	77	77	60	60	266	266	77	478	478	100
Composition, mass fraction										
Adipic Acid	1	0	0	0	0.556	0.556	0	0	0	0
Hexamethylenediamine (HMDA)	0	1	0	0	0.442	0.442	0	0	0	0
Water	0	0	1	1	0.002	0.002	0	1	0.002	0.002
Nitrogen	0	0	0	0	0	0	1	0	0	0
Nylon-6,6	0	0	0	0	0	0	0	0	0.998	0.998
Mass Flow Rate (lb/day)	167,095	132,872	1,390	1,390	301,357	301,357	1,477	42,150	259,271	259,271
Density (lb/ft3)	84.9	52.4	62.4	62.4	66.6	66.6	0.21	0.51	71.79	71.2

Figure 6: Stream Summary Table

Process Description

In this process, Adipic Acid and HMDA are mixed to form Nylon-6,6 and water. The reactants are dissolved, heated, and stirred in a mixer to form a dissolved salt solution, then flow to a polymerization reactor. Upon entering this reactor, the dissolved salt begins to form Nylon-6,6 and water. Heat is added to evaporate the product water, which is then vented to the atmosphere, thus driving the reaction forward. Once the water content in the product reaches 0.2% by mass, the molten Nylon-6,6 product is extruded, cut, and cooled, then packaged and stored for sale.

This process manufactures Nylon-6,6 in four batches per day, with each batch taking approximately six hours to complete. The designed production facility includes five mixers and five polymerization reactors. This number was selected so that four mixer/reactor pairs could be used at any given time, and the fifth pair could be offline for service and cleaning. The reactors will be switched every other day, so that each pair will operate for a maximum of eight consecutive days between cleanings. This time cycle can be adjusted to account for more or less cleaning time if needed. The mixers and reactors were sized to include a safety factor of 0.75, thus reducing the likelihood of overflow. Each mixer and reactor has a volume of 452 ft³ and 481 ft³, respectively. The layout of the mixers and reactors can be found in the PFD, on pages 10 and 11.

All mixers and reactors are agitated and jacketed, and all utilize electric heating. Electric heating was selected over using steam or fired heating by considering local utility costs for water (and water treatment), fuel gas, and electricity.^{6,16,19} The price of electricity for Calvert City makes electric heating an affordable energy cost. Use of electricity minimizes the amount of equipment needed to heat the process. It is assumed that the mixers, reactors, and pipes are well-insulated, and thus any heat lost by the system during production is negligible.

The reactants for production of Nylon-6,6 are stored in tanks at the manufacturing facility. Because HMDA is a hazardous substance, the tanks are sealed and the process for loading the mixers is automated, thus lessening the risk posed to operators handling the materials. Temperature indicators are installed on every tank due to the flammability hazards associated with the Adipic Acid and HMDA. Because of the corrosive nature of the reactants, the storage tanks are both made of stainless steel. The tanks are raised higher than the inlet to mixers so that the reactants may be loaded to the mixers using gravity. The storage tanks for each of the two reactants are each capable of holding two days' worth of production material when the process is operating at full-scale. The cost of purchase and transport of raw material into the plant is accounted for in the annual operating cost of the process.

Water is needed to dissolve the Adipic Acid and HMDA in the mixer to form a salt solution of ions. The water is purchased, treated, and stored in one carbon steel tank that is also capable of holding two days' worth of water needed for production. The storage tanks for the water, the Adipic Acid, and the HMDA are sealed tanks at atmospheric pressure. The equipment sheets for the storage tanks can be found on pages 25, 26, and 27.

The first step in the process is to load the HMDA and Adipic Acid into the mixers being utilized for the current batch. As mentioned, four of the five mixer/reactor pairs are in operation during any given batch, with the last pair out of service for cleaning and maintenance. Equivalent amounts of Nylon-6,6 are produced in each of the pairs in service. Equivalent stoichiometric amounts of Adipic Acid and HMDA are loaded into each mixer. The amount of each substance added to the reactor is controlled by a scale that measures the weight of the contents in the mixer. The water needed to dissolve the reactants is pumped to each mixer at 40 psi. The mixer is stirred and heat is added until the contents reach a temperature of 266°F, which is the solubility temperature of the reactants in the given amount of water. Because this temperature is well above the boiling point of water at atmospheric pressure, additional water is added to the mixer to pressurize it to the saturation pressure of water at 266°F. The mixer pressure becomes approximately 40 psi as the water is vaporized.

The amount of each reactant and water required during each batch and per mixer is shown in Table 2, below.

Table 2: Material Required for One Cycle

Material	Amount Per Batch (lb)
Adipic Acid	41,774
HMDA	33,218
Water	348

The amount of heat added to the reactor is controlled by a temperature indicator and controller on each mixer. The set point for the temperature of the mixer contents is set to 266°F and heat is added until that temperature is reached. At this point, all reactants are dissolved in solution and the formation of steam has pressurized the reactor. The mixer is equipped with a relief valve that will automatically release in the case of overpressure.

Before the contents of the mixer can be transferred to the polymerization reactor, the reactor is purged with nitrogen. This is done to eliminate the presence of any oxygen in

the reactor which might cause degradation of the Nylon-6,6 product. The nitrogen is supplied to the four reactors in use from a nitrogen delivery source and is released through a relief valve on the reactors. Approximately 370 lbs of nitrogen are needed per reactor per cycle, and the nitrogen is fed to the reactor at 20 psi. This is a great enough pressure to exit the reactor and vent to atmosphere as well as a small enough pressure for the mixer contents to enter the reactor without the use of a pump.

Table 3: Nitrogen Requirement

Material	Amount Per Batch (lb)
Nitrogen	1480

Once the nitrogen purge on the reactor is complete and the reactants are fully dissolved into the intermediate salt solution at 266°F, they are immediately loaded into the reactor. (Note: It is assumed that no Nylon-6,6 product is formed in the mixer for the preliminary design of this process.) There is a check valve on the line between the mixer and the reactor to prevent backflow into the mixer. Once the solution is transferred to the reactor, heat is continually added until the temperature is 478°F. At this temperature, the nylon is in a molten form and can be extruded. The temperature is monitored with a temperature indicator; a control is in place to add heat until the desired temperature is reached. The pressure in the reactor is then allowed to decrease to atmospheric pressure by venting steam to the atmosphere. As this happens, the water byproduct produced in the reaction between Adipic Acid and HMDA evaporates, thus driving the reaction further towards the product side. The reactor is stirred and heat is added to continue the evaporation of the water until the water content is less than 0.2% by mass. This process is controlled by measuring the amount of steam venting to the atmosphere with a flow indicator.

Simulation data indicated that reaction time is 4-6 hours.³⁰ Using this information, a kinetic simulation for the reaction was completed using PolyMath software. The results from this simulation are found in the Appendix on pages 77 and 78. The following figure graphically represents conversion as reaction time progresses.

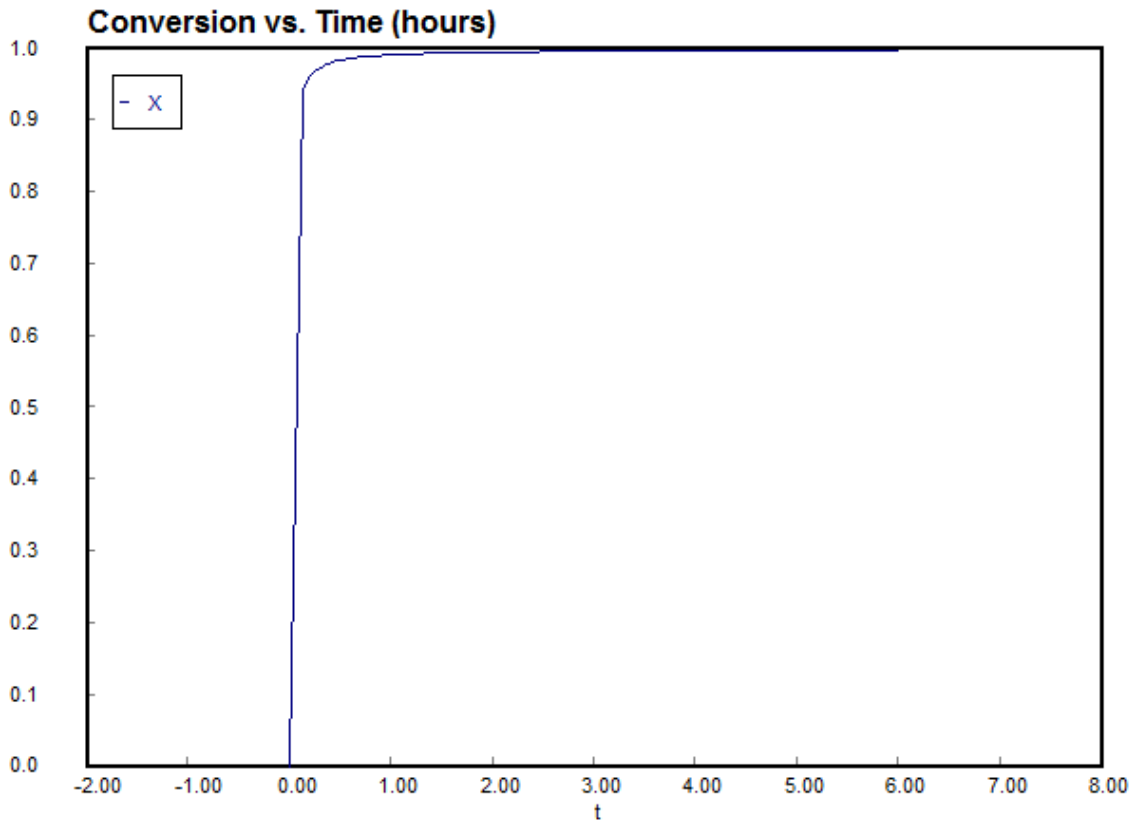


Figure 7: Conversion vs. Time for Nylon-6,6 Reaction

Based on the Figure 7, a conversion of 100% was assumed and the total time per batch, including mixing, reacting, and extruding, was determined to be six hours.

The molten Nylon-6,6 is pressurized out of the reactors using the nitrogen purge for the next cycle. The nylon product from all four reactors in use is combined and extruded. As the formed strands leave the extruder, they are cut into chips and are deposited onto a conveyor. Cooling water passes over chips as they move along the conveyor to cool them to a temperature of approximately 100°F. A fan continues to cool and dry the chips during the remainder of the conveyor residence time. The chips are packaged into bags that are sealed and stored for sales. During further stages of design and depending on the main mode of transportation of the product, methods to deposit the sealed packages directly into rail cars, semi-trucks, or other modes of transportation should be evaluated.

Energy Balance and Utility Requirements

The energy requirements for this process were derived from an energy balance performed around the two central pieces of equipment, the mixer and the polymerization reactor. Energy requirements also include the necessity of cooling water to cool the

extruded product. The equations used to calculate energy requirement for each piece of equipment can be found on page 55 in the Appendix.

Mixer

The first step in the process is forming a salt solution of water, Adipic Acid, and HMDA in the mixer. Solubility of the reactants was taken into consideration when determining how much water is necessary to form a solution. A lesser amount of water requires less purchase cost, but must be heated to a higher temperature to dissolve the reactants. The solubility of Adipic Acid was used as a limiting reagent because HMDA has a greater solubility in water. An energy balance was performed to determine the amount of energy required to increase the temperature of the water, and therefore the solubility of the reactants. The costs of water and energy were compared in order to determine the optimal volume of the water and water temperature with which to dissolve the reactants. After optimization it was determined that a smaller volume of water required less energy input, even when heated to a higher temperature. The results from this optimization are in the Table 25 on page 63 in the Appendix. This optimization does not include the amount of water added to pressurize the mixer or the energy to heat the solid HMDA or Adipic Acid, but as these values are nearly constant, the cost comparison is not impacted significantly. The energy requirement and cost for heating the contents of the four mixers is listed below in Table 4. Electricity is the utility used to heat the mixers.

Table 4: Energy Demand for Mixer Heating

Q_{mixer} (Btu/hr)	2,611,534
Cost of Mixer Heating (\$/year)	\$387,000

There is an agitator in the mixer in order to increase solubility and produce a well-mixed solution. The cost for mixing was calculated as 75% of the cost of heating. From this assumption, the energy requirement of the four mixers was calculated. Electricity is used for agitation. The results are listed in the table below.

Table 5: Energy Demand for Mixer Agitation

$Q_{\text{mixer,agitator}}$ (Btu/hr)	1,958,650
Cost of Mixer Agitation (\$/year)	\$291,000

Polymerization Reactor

The formation of Nylon-6,6 from Adipic Acid and HMDA is an endothermic reaction, and as such requires heat to proceed. The contents of the reactor are heated from a temperature of 266°F to a temperature of 478°F. This maximum temperature is set based on the melting point of Nylon-6,6 and the need for a molten form of the product for extrusion. An energy balance was performed around the polymerization reactor and accounts for heat absorbed by the reaction. The energy requirement and cost for heating the reactor is listed below in Table 6. The utility used to heat the reactors is electricity.

Table 6: Energy Demand for Reactor Heating

Q_{reactor} (Btu/hr)	2,580,420
Cost of Reactor Heating (\$/year)	\$383,000

There is an agitator in the polymerization reactor to increase polymerization of Nylon-6,6.²⁴ The cost for agitation was calculated in manner consistent with that of the mixer agitation. Electricity is again used for agitation.

Table 7: Energy Demand for Reactor Agitation

$Q_{\text{reactor,agitator}}$ (Btu/hr)	1,935,316
Cost of Reactor Agitation (\$/year)	\$287,000

The formation and release of steam creates a possibility for heat integration in this design. The major focus area for heat integration is using the steam to preheat the water prior to entering the mixer. This reduces operating costs and energy requirements for the mixing process. Although the amount of steam is sufficient to heat the water to the selected temperature of 266°F, heat integration was rejected for this design. Because a batch process was selected, the timing of the release of steam is not compatible with the timing of the water fed to the mixer. The release of steam from the polymerization reactor occurs when driving the reaction to completion, in the latter half of the process. This release occurs before another batch begins in the mixer. After heat integration was rejected, the possibility of material integration was considered. The idea of condensing the steam, treating it, and recycling to use as feed water was explored. A heat exchanger with a cooling water utility was designed to condense the steam. The operating cost of the heat exchanger was on the order of millions of dollars per year due to the volume of steam condensed per day. The expense of operating this heat exchanger would outweigh the cost of purchasing treated water for the process. The results from the water integration calculations can be seen on page 64 in the Appendix.

An energy balance was performed to determine the amount of cooling water necessary to cool the Nylon-6,6 product in order to prepare for sale. The product is cooled from the temperature of 478°F, at the outlet of the polymerization reactor to a temperature of 100°F. The cooling water supply and return temperatures of 60°F and 102°F respectively were used in the energy balance calculation.¹⁴

Below is a summary of the energy demands for the process and the sources of those demands.

Table 8: Summary of Energy Demands for the Process

<i>Energy Demands</i>
2,611,534 Btu/hour to heat the contents mixer from 60°F to 266°F
2,580,420 Btu/hour to heat the contents of the reactor from 266°F to 478°F
73,531,718 Btu/hour to heat cooling water from 60°F to 102°F

Table 9: Summary of Sources of Energy Demands

<i>Source of Energy Demands</i>
2,611,534 Btu/hour from power generator to heat mixer
2,580,420 Btu/hour from power generator to heat reactor
73,531,718 Btu/hour from extruded Nylon-6,6 product as it cools from 478°F to 100°F

Equipment List and Unit Specifications

Mixer and Polymerization Reactors

Mixers M-1 through M-5 and polymerization reactors PR-1 through PR-5 were sized using a combination of material balances, energy balances, safety considerations, and by optimization. An overall mass balance was performed to determine the amount of material entering the mixer. These equations can be seen on page 54 in the Appendix. Detailed energy balance calculations for the mixers and the polymerization reactors can be seen on page 61 in the Appendix. The process was optimized for two conditions: number of cycles per day and number of reactors per cycle. Four cycles per day was selected over three cycles and two cycles per day because running four cycles per day would result in smaller reactor volume thus reducing the capital cost of the reactors as seen on pages 68 and 70 in the Appendix. An optimization was also performed on the number of mixers and reactors versus present worth cost however, this optimization was inconclusive as the results showed a nearly linear relationship, as seen on page 97 in the Appendix. Because of the inconclusive optimization, the number of mixers and

reactors were chosen in order to accommodate the variation in capacity and for safety and loss prevention concerns. In order to easily change capacities, four mixers and reactors were selected with an additional fifth mixer and reactor for sparing purposes. In total, five mixers and five polymerization reactors were included in this design. The fifth mixer and reactor allow for equipment to be rotated every other day for cleaning and maintenance purposes. Each mixer and reactor will be constructed from stainless steel as Adipic Acid and HMDA will corrode other standard materials of construction. The volume of the mixers are 452 ft³ and the volume for the polymerization reactors is 481 ft³. The mixer equipment specification sheet can be seen on page 29 and the detailed mixer cost estimate can be seen on page 73 in the Appendix. The cost of each mixer is \$270,000. The polymerization reactor equipment specification sheet can be seen on page 30 and the detailed reactor cost estimate can be seen on page 73 in the Appendix. The cost of each reactor is \$280,000.

Feed Water Pumps

Feed water pump P-100A was sized to supply five horsepower (hp) using the hydraulic pump sizing equation on page 56 in the Appendix. Detailed calculations for the pump can be seen on page 71 in the Appendix. The cost each pump is \$17,000. This design includes two pumps with one of the pumps (P-100B) acting as a spare. As these pumps will be used strictly for feed water, they will be constructed out of carbon steel as there is no corrosion concern. The pump equipment specification sheet can be seen on page 28.

Storage Tanks

The tanks T-100A/B, T-101A/B, and T-102 were sized to accommodate a reasonable amount of reactant storage. The HMDA storage tanks (T-100A/B) and the Adipic Acid storage tanks (T-101A/B) were sized to hold two days' worth of reactants each. Overall, the plant will have enough Adipic Acid and HMDA stored to run the process for four days. All four of these tanks will need to be constructed out of stainless steel to prevent corrosion from HMDA and Adipic Acid. The volume of each HMDA tank in this design is 5072 ft³ and the volume of each Adipic Acid tank is 3936 ft³. Since water is more readily available than both HMDA and Adipic Acid, only one feed water storage tank (T-102) will be present which can hold two days' worth of feed water. The feed water tank material of construction is carbon steel and the tank has a volume of 20.7 ft³. The Adipic Acid storage tank equipment specification sheet can be seen on page 26 and the detailed cost estimate can be seen on page 72 in the Appendix. The cost of each Adipic Acid storage tank is \$802,000. The HMDA storage tank equipment specification sheet can be seen on page 25 and the cost estimate can be seen on page 72 in the Appendix. The cost of each HMDA storage tank is \$402,000. The feed water storage tank equipment specification sheet can be seen on page 27 and the cost estimate can be seen on page 74 in the Appendix. The cost of the water storage tank is \$367,000.

Extruder and Packager

The Extruder and Packager (E-100) was sized using the mass balance seen on page 69 in the Appendix. The extruder and packager material of construction is stainless steel and the volume is 1236 ft³. The equipment specification sheet can be seen on page 31 and the detailed cost estimate can be seen on page 73 in the Appendix. The cost of the extruder and packager is \$565,000.

There were difficulties encountered when sizing the extruder and packager. The extruder was sized according to procedures in Reference 34 for sizing a pressure vessel. To account for the additional extrusion equipment on the vessel as well as the packager, an additional factor of two was taken into account as seen on page 73 in the Appendix.

Conveyor

The Conveyor (C-100) was sized from the mass of Nylon-6,6 per cycle in order to account for all the material the conveyor cools per cycle. The conveyor is constructed from carbon steel and silicone as pellets of Nylon-6,6 do not pose a risk of causing corrosion to carbon steel. The length of the conveyor belt is sized to be 328 ft and the width of the conveyor is 3.28ft. The surface area for Nylon-6,6 pellets to cool and dry on is 538.2 ft². While on the conveyor, 64,818 pounds of Nylon-6,6 will be cooled in order to be packaged and shipped. The equipment specification sheet can be seen on page 32 and the detailed cost estimate can be seen on page 73 in the Appendix. The cost of the conveyor is \$271,000.

A summary of the unit types, equipment numbers, and operating conditions can be found on the next page.

Table 10: Equipment Summary Table

Unit Numbers	Unit Type	Brief Function Description	MOC	Size	Operating Temperature	Operating Pressure
P-100 A/B	Centrifugal Pump	Pumps water from T-102 to mixers M-1 through M-5	Carbon Steel	5 hp	60F	N/A
M-1, M-2, M-3, M-4, M-5	Mixer	Mixes HMDA, AA, and water and heats the solution to 266F	Stainless Steel	452 ft3	266F (max)	40 psia
PR-1, PR-2, PR-3, PR-4, PR-5	Polymerization Reactor	Vessel where the polymerization of the HMDA/AA solution occurs	Stainless Steel	481 ft3	478F (max)	270 psia (max)
T-100 A/B	HMDA Storage Tank	Storage tank for two days worth of reactant HMDA	Stainless Steel	5072 ft3	77F	14.7 psia
T-101 A/B	AA Storage Tank	Storage tank for two days worth of reactant AA	Stainless Steel	3936 ft3	77F	14.7 psia
T-102	Feed Water Tank	Storage tank for two days worth of feed water	Carbon Steel	20.7 ft3	60F	14.7 psia
E-100	Extruder	Extrudes molten Nylon-6,6 into pellets and packages into sealed bags after cooling	Stainless Steel	1236 ft3	478F (max)	43.7 psia
C-100	Conveyor	Transports Nylon-6,6 pellets while cooling before being packaged	Silicone and Carbon Steel	1075 ft2	478F (max)	14.7 psia

Equipment Specification Sheets

The equipment specification sheets can be found on the following pages for each piece of equipment in the process.

HMDA STORAGE TANK		
Identification:	Item No.	T-100A/B
	No. Required	2
Function:	HMDA Storage Tank	
Operation:	Batch	
Materials Handled:	HMDA	
Volume	5072 ft ³	
Holding Capacity	265,744 lb HMDA	
Component Mass Fractions:		
<i>AA</i>		0.0
<i>HMDA</i>		1.0
<i>Water</i>		0.0
<i>Nylon-6,6</i>		0.0
Temperature (F):		77
Design Data:	Material of Construction	Stainless Steel
	Operating Pressure	14.7 psi
	Design Pressure	14.7 psi
	Volume	5072 ft ³

Figure 8: HMDA Storage Tank Equipment Specification Sheet

ADIPIC ACID STORAGE TANK		
Identification:	Item No.	T-101A/B
	No. Required	2
Function:	Adipic Acid Storage Tank	
Operation:	Batch	
Materials Handled:	Adipic Acid	
Volume	3936 ft ³	
Holding Capacity	334,190 lb AA	
Component Mass Fractions:		
<i>AA</i>		1.0
<i>HMDA</i>		0.0
<i>Water</i>		0.0
<i>Nylon-6,6</i>		0.0
Temperature (F):		77
Design Data:	Material of Construction	Stainless Steel
	Operating Pressure	14.7 psi
	Design Pressure	14.7 psi
	Volume	3936 ft ³

Figure 9: Adipic Acid Storage Tank Equipment Specification Sheet

FEED WATER STORAGE TANK		
Identification:	Item No.	T-102
	No. Required	1
Function:	Feed Water Storage Tank	
Operation:	Batch	
Materials Handled:	Adipic Acid	
Volume	20.7 ft ³	
Holding Capacity	2,780 lb Water	
Component Mass Fractions:		
<i>AA</i>		0.0
<i>HMDA</i>		0.0
<i>Water</i>		1.0
<i>Nylon-6,6</i>		0.0
Temperature (F):		60
Design Data:	Material of Construction	Carbon Steel
	Operating Pressure	14.7 psi
	Design Pressure	14.7 psi
	Volume	20.7 ft ³

Figure 10: Feed Water Storage Tank Equipment Specification Sheet

FEED WATER PUMP		
Identification:	Item	Feed Water Pump
	Item No.	P-100A/B
	No. Required	2 (spared)
Function:	Pump feed water to 40 psig to be sent to the mixer.	
Operation:	Continuous while water is fed to mixer.	
Materials Handled:	Suction	Discharge
Quantity (lb/cycle):	161.59	161.59
Component Mass Fraction:		
Water	1.0	1.0
Pressure (psig):	14.7	40
Design Data:	Temperature	60 F
	Material of Construction	Carbon Steel

Figure 11: Feed Water Pump Equipment Specification Sheet

REACTANT MIXER					
Identification:	Item	Mixer			
	Item No.	M-1 through M-5			
	No. Required	5			
Function:	Mix Adipic Acid (AA), Hexamethylenediamene (HMDA), and water at 266 degrees Fahrenheit. Each mixer runs four cycles per day.				
Operation:	Batch				
Materials Handled:	Inlet, Water	Inlet, AA	Inlet, HMDA	Outlet	
Quantity (lb/cycle/mixer):	162	41774	33218	75153	
Component Mass Fractions:					
<i>AA</i>	0.0	1.0	0.0	0.556	
<i>HMDA</i>	0.0	0.0	1.0	0.442	
<i>Water</i>	1.0	0.0	0.0	0.002	
<i>Nylon-6,6</i>	0.0	0.0	0.0	0.0*	
Temperature (F):	60	77	77	266	
Design Data:	Material of Construction	Stainless Steel			
	Operating Pressure	40 psi			
	Design Pressure	90 psi			
	Volume per Mixer	452 ft ³			
	Height	4 ft			
	Diameter	11.5 ft			
	Agitated?	Yes			
	Baffles?	Yes			
*Note: A small amount of Nylon-6,6 may be present as the reaction may begin once the reactants dissolve in water and become a dissolved salt.					

Figure 12: Reactant Mixer Equipment Specification Sheet

POLYMERIZATION REACTOR						
Identification:	Item	Reactor				
	Item No.	PR-1 through PR-5				
	No. Required	5				
Function:	Produce Nylon-6,6 and Water from Adipic Acid (AA) and Hexamethylenediamine (HMDA). Heat the contents of the reactor to evaporate water to meet Nylon-6,6 product specification.					
Operation:	Batch					
Materials Handled:	Inlet, Nitrogen	Inlet, Mixed Reactants	Outlet, Nitrogen	Outlet, Steam	Outlet, Nylon-6,6 Product	
Quantity (lb/cycle):	369.2	75153.34	369.2***	10351.5	64817.6	
Comp. Mass Fractions:						
<i>AA</i>	0	0.556	0	0	0	
<i>HMDA</i>	0	0.442	0	0	0	
<i>Nitrogen</i>	1	0	1	0	0	
<i>Water</i>	0	0.002*	0	1	0.002	
<i>Nylon-6,6</i>	0	0**	0	0	0.998	
Temperature (F):	77	266	77	478	478	
Design Data:	Material of Constuction	Stainless Steel				
	Operating Pressure	270 psi (max)				
	Design Pressure	320 psi				
	Volume per Mixer	481 ft3				
	Height	4.25 ft				
	Diameter	12 ft				
	Agitated?	Yes				
	Baffles?	Yes				
*Slightly more water may be present in the inlet feed, as water is a product of the reaction between AA and HMDA.						
**A small amount of Nylon-6,6 may be present as the reaction may begin once the reactants dissolve in water and become a dissolved salt.						
***There may be a small amount of nitrogen left once the tank is purged. This small amount will be cleared when the steam begins to evaporate.						

Figure 13: Polymerization Reactor Equipment Specification Sheet

EXTRUDER			
Identification:	Item	Extruder and Packager	
	Item No.	E-100	
	No. Required	1	
Function:	Extrude, cut, and cool product Nylon-6,6 and package finished product chips.		
Operation:	Batch		
	Inlet, Molten		Outlet, Product
Materials Handled:	Nylon	Cooling Water	Chips
Quantity (lb/cycle):	64,818	459,573	64,818
Comp. Mass Fractions:			
<i>Adipic Acid</i>	0	0	0
<i>HMDA</i>	0	0	0
<i>Water</i>	0.002	1	0.002
<i>Nylon-6,6</i>	0.998	0	0.998
Temperature (F):	478	60	100*
Design Data:	Material of Construction	Stainless Steel	
	Extruder Type	Screw	
	Packaging Type	Bag	
	Pressure	43.7 psia	
	Volume	1236 ft ³	
*Finished Nylon-6,6 product will continue to cool as it moves along conveyor belt and is packaged.			

Figure 14: Extruder Equipment Specification Sheet

CONVEYOR			
Identification:	Item	Conveyor	
	Item No.	C-100	
	No. Required	1	
Function:	To transport and cool the Nylon-6,6 product coming from the extruder.		
Operation:	Batch		
Materials Handled:	Inlet, Molten Nylon	Cooling Water	Outlet, Product Chips
Quantity (lb/cycle):	64,818	459,573	64,818
Comp. Mass Fractions:			
<i>Adipic Acid</i>	0	0	0
<i>HMDA</i>	0	0	0
<i>Water</i>	0.002	1	0.002
<i>Nylon-6,6</i>	0.998	0	0.998
Temperature (F):	478	60	100*
Design Data:	Material of Construction	Silicone, CS	
	Pressure	14.7 psi	
	Area	1075 ft ²	
<p>Note: The conveyor, packager, and extruder are part of the same mechanism and the conveyor is located between the extruder and packager.</p> <p>*Finished Nylon-6,6 product will continue to cool as it moves along conveyor belt and is packaged.</p>			

Figure 15: Conveyor Equipment Specification Sheet

Equipment Cost Summary

The following table summarizes the estimated purchase cost of each piece of equipment used in the process. The costs were estimated using costing correlations outlined in Reference 34.

Table 11: Equipment Cost Summary Table

Equipment	Unit Numbers	Unit Type	Cost per Unit	Number Purchased	Total Cost
Mixing Reactor	M-1, M-2, M-3, M-4, M-5	Jacket, Agitated	\$270,000	5	\$1,350,000
Polymerization Reactor	PR-1, PR-2, PR-3, PR-4, PR-5	Jacket, Agitated	\$280,000	5	\$1,400,000
Water Feed Pump	P-100 A/B	Centrifugal	\$17,000	2	\$33,000
Adipic Acid Storage Tank	T-100 A/B	Fixed Roof	\$802,000	2	\$1,610,000
HMDA Storage Tank	T-101 A/B	Fixed Roof	\$402,000	2	\$804,000
Feed Water Tank	T-102	Fixed Roof	\$367,000	1	\$367,000
Extruder and Packager	E-100	Screw Extruder	\$565,000	1	\$565,000
Conveyor	C-100	Belt	\$271,000	1	\$271,000

Fixed Capital Investment Summary

The total installed cost of the production equipment, as well as the grassroots cost of the production facility can be seen in Table 12, below.

Table 12: Fixed Capital Investment Summary

Total Installed Cost	\$6,400,000
Total Grass Roots Cost	\$10,800,000

The fixed capital investment for this process was estimated using procedures outlined in Reference 34 to cost each piece of equipment. In order to cost equipment for a

grassroots plant, the total fixed capital investment was multiplied by a factor of as seen on page 58 in the Appendix.

Mixing and Polymerization Reactors

Detailed calculations for the cost of Mixers M-1 through M-5 can be seen on page 73 in the Appendix and detailed calculations for the cost of Polymerization Reactors PR-1 through PR-5 can be seen on page 73 in the Appendix.

Feed Water Pumps

Detailed calculations for the cost of Feed Water Pumps P-100A/B can be seen on page 74 in the Appendix.

Storage Tanks

Detailed calculations for the cost of reactant Storage Tanks T-100A/B, T-101A/B, and T-102 can be seen on page 72 in the Appendix.

Extruder and Packager

Detailed calculations for the cost of Extruder and Packager E-100 can be seen on page 73 in the Appendix.

Conveyor

Detailed calculations for the cost of Conveyor C-100 can be seen on page 73 in the Appendix.

Safety, Health, and Environmental Considerations

1. Chemical Safety and Environmental Concerns

The reaction chemistry for the production of Nylon-6,6 involves the use of different compounds that have the potential to be hazardous to both personnel and the environment. Safety Data Sheets for each chemical compound can be found on pages 81 through 96 in the Appendix. Understanding the potential hazards and developing an effective plan helps to mitigate the risk of environmental and personal harm from the chemicals used in the production of Nylon-6,6. An analysis of the hazards and a mitigation plan has been evaluated for the preliminary design process. Care has been taken to minimize the risk posed by the use of hazardous materials and severe operating conditions.

Hexamethylenediamine

HMDA is a reactant in the production process and has many hazardous characteristics. HMDA is a combustible compound and should never come in contact with open flames to prevent combustion. Fires caused by HMDA combustion can be extinguished with

powder, alcohol-resistant foam, large amounts of water, or with carbon dioxide. HMDA should be stored in a well-sealed, unbreakable container in order to avoid contact with strong acids and strong oxidants. This type of storage helps prevent the spillage of HMDA which is toxic to aquatic life. Because of this, HMDA should never be released into the environment.¹²

Adipic Acid

The second reactant in this process is Adipic Acid. Adipic Acid is a combustible compound and should be stored away from open flames. A fire caused by the combustion of Adipic Acid can be extinguished using powder, water spray, foam, or Carbon Dioxide. Particles of Adipic Acid in the air can create an explosive mixture. To prevent explosions, dust explosion-proof electrical equipment should be used throughout the polymerization plant. Particle explosions can also be ignited by the discharge of static electricity which can be prevented by grounding. Like HMDA, Adipic Acid is harmful to aquatic life and releases into water sources should be prevented. Acceptable ways to dispose of Adipic Acid are by landfill, incinerator, or recycle.¹

Nylon-6,6

For this process, Nylon-6,6 will be produced as small, solid pellets. The major safety concern with pellets is that pellets can become a slipping hazard when spilled. While Nylon-6,6 is not combustible or explosive, burning Nylon-6,6 can produce a dense, toxic smoke which could contain ammonia, carbon monoxide, and small amounts of hydrogen cyanide and aldehydes. Burning Nylon-6,6 can be extinguished using water, foam, or Carbon Dioxide. The preferred disposal methods for Nylon-6,6 are recycling, incineration with an energy recovery, and by landfill.²¹

Nitrogen

Nitrogen is used in this process in order to purge the polymerization reactor. While Nitrogen is not combustible, heating Nitrogen will result in a rise in pressure which risks bursting process equipment. Compressed Nitrogen should be kept in a cool, well-ventilated room preferably in a fireproof building or room. The amount of Nitrogen used throughout this process is small enough that any effects from venting to atmosphere are negligible.²³

2. Chemical Health Concerns

While each of these compounds also pose significant health hazards, health risks can be mitigated through proper safety procedures.

Hexamethylenediamine

If inhaled, HMDA can cause a burning sensation, labored breathing and shortness of breath, sore throat, and cough. In order to prevent the side effects associated with

inhaling HMDA, facilities should be equipped with ventilation systems, local exhaust, and have breathing protection readily available. The treatment for the inhalation of HMDA consists of supplying the afflicted person with fresh air, rest, and artificial respiration, if needed. HMDA can be absorbed through skin and absorption will result in redness, burns, blisters, and pain. To prevent direct skin contact, personnel should wear protective gloves and clothing. If direct skin contact occurs, the affected area should be rinsed with water. Eye exposure to HMDA, which can be prevented with the proper safety glasses and face shields, can cause redness, pain, and burns. Eye exposure should be treated by rinsing the eyes with plenty of water for several minutes; medical attention should be given after rinsing is completed. Ingestion of HMDA results in abdominal cramps, pain, burning, and/or collapse and afflicted personnel should be referred to medical professionals immediately.¹²

Adipic Acid

Adipic Acid can cause coughing and sore throat when inhaled. To prevent inhalation, facilities should be equipped with a local exhaust system. Protective clothing and gloves should always be worn when dealing with Adipic Acid. If direct skin contact with Adipic Acid occurs, contaminated clothing should be removed and affected areas should be rinsed with water. Safety glasses or other similar eye protection should be worn by all personnel to avoid redness and pain caused by eye contact with Adipic Acid.¹

Nylon-6,6

Molten Nylon-6,6 produces fumes that can cause eye and skin irritation as well as breathing problems. To avoid potential problems caused by fumes, facilities should be well ventilated and molten Nylon-6,6 should be contained in closed vessels. If molten Nylon-6,6 comes in contact with skin, it will cause severe burns. If contact occurs, the polymer should be cooled with water and medical attention should be sought in order to remove the cooled Nylon-6,6 from skin. Nylon-6,6 in pellet form poses no significant health risks.²¹

Nitrogen

Large concentrations and accidental releases of Nitrogen in enclosed spaces can result in lowered oxygen concentrations which can cause unconsciousness, weakness, and, in extreme cases, suffocation. All facilities using Nitrogen need to be equipped with ventilation systems.²³

3. Plant Safety Plan

Considering the numerous health and environmental concerns associated with each of the chemicals involved in this process, it is imperative to have an effective safety and risk mitigation plan put in place. The biggest hazard with this process is the potential of fire outbreaks due to the flammable nature of HMDA. To help prevent major damage by

fires, temperature indicators will be installed on both the HMDA and Adipic Acid storage tanks. These indicators will help operators mitigate the risk of fire by cooling the storage vessels with water to reduce the chance of combustion. If a fire were to occur, the facility will be equipped with a deluge system as well as alcohol-resistant foam systems. To mitigate risk to personnel, a siren system will be utilized to alert employees of dangerous conditions including fires. Muster points will also be considered in the planning stage to ensure there will be safe locations for employees to meet away from immediate risk. The control room will be built with blast proof walls to reduce the chance of injury to essential process operators.

The facility will have a dedicated emergency response team made up of plant employee volunteers. The team will have frequent meetings and trainings to ensure that they are prepared in case of an accident. The team will also coordinate with the local emergency services. In case of emergency, all employees will understand protocol necessary to mitigate potential consequences.

Due to the hazards associated with inhalation of any of the chemicals involved in this production process, ventilation systems will be installed throughout every building in the plant. Gas detection sensors will also be installed to further protect employees in the case of a ventilation system failure.

The preliminary control scheme on equipment involves the use of pressure, temperature, flow, and level indicators. The temperature and pressure indicators on all mixers and polymerization reactors are critical instruments. These critical instruments will be associated with numerous alerts and alarms as well as emergency shutdown (ESD) procedures. Each mixer and reactor will also be equipped with pressure relief valves to mitigate the risk of over pressuring a vessel.

Process Controllability and Instrumentation

The first location in the process the chemicals interact is in the mixers. The addition of Adipic Acid and HMDA is controlled by a scale on each mixer to ensure that there is an equimolar amount of each reactant. This is important because excess of either reactant will lead to unreacted material in the polymerization reactor, which will then decrease the purity of the Nylon-6,6 product. Water is not added until both of the dry reactants are added. Water is measured going into the mixer using a level transmitter so that the correct amount is added to dissolve the reactants. If too little water is used, not all of the reactants will dissolve. If too much water is added, operating costs increase because more energy is required to evaporate the water.

Heat is added to the mixer to increase solubility of the reactants, and the amount of heat added is controlled by a temperature transmitter. As the mixer is heating, steam is produced and pressurizes the vessel. If too much heat is added the vessel will over pressurize and a relief valve will be utilized.

A nitrogen purge is used to eliminate any presence of oxygen from the polymerization reactor prior to loading. The amount of nitrogen added to the reactor is monitored through a flow transmitter and does not pose any significant risk of overpressure. The nitrogen will be released through a relief valve on the reactor as the dissolved salt intermediate is loaded, and the remainder of the nitrogen will be driven out by evaporating steam from the process.

The temperature and pressure of the polymerization reactor are measured using a temperature and pressure transmitter, respectively. The measured pressure inside the reactor is linked to a control valve on the relief system, thus adjusting the rate of steam exiting the reactor at any point during the reaction.

Operating Cost

Per Reference 34, overall manufacturing cost is generally a function of capital costs and raw material purchase. The following manufacturing costs are associated with production of Nylon-6,6. Maintenance cost is a function of capital cost and is included in annual operating cost. Operating labor is a function of the number of pieces of equipment in the plant; for this process seven operators are required annually. Clerical and supervisory labor costs and laboratory charges are functions of operating labor costs. Operating supplies costs are a function of capital investment. Overhead costs are also a function of operating labor costs and capital costs. The estimated annual operating costs for the production of Nylon-6,6 are summarized in the following cost sheets. A cost sheet for operation at 100% capacity and operation at 67% are included, on pages 39 and 40 respectively.

Table 13: Cost Sheet - 100% Capacity

Raw Materials		
	Adipic Acid	\$0.61/lb
	Hexamethylenediamine	\$1.12/lb
	Water	\$0.00106/lb
	Nitrogen	\$0.0033/lb
<i>Total Raw Material Cost/year</i>		\$82,500,000
Utilities		
	Electricity	\$0.0545/kWh
	Cooling Water	\$3.85/100 gallons
<i>Total Utility Cost/year</i>		\$3,230,000
Water Treatment		\$0.0006/lb
<i>Total Water Treatment Cost/year</i>		\$8,300
Operating Labor		
	Direct Supervisory and Clerical Labor	\$410,000
	Maintenance and Repairs	\$74,000
	Operating Supplies	\$643,000
	Laboratory Charges	\$97,000
<i>Total Direct Manufacturing Costs</i>		\$87,000,000
Local Taxes and Insurance		
	Plant Overhead Costs	\$343,000
<i>Total Fixed Manufacturing Costs</i>		\$676,000
Total Cost of Production Cost		\$88,100,000
Cost of Nylon-6,6		\$1.04/lb

Table 14: Cost Sheet - 67% Capacity

Raw Materials		
	Adipic Acid	\$0.61/lb
	Hexamethylenediamine	\$1.12/lb
	Water	\$0.00106/lb
	Nitrogen	\$0.0033/lb
<i>Total Raw Material Cost/year</i>		\$55,300,000
Utilities		
	Electricity	\$0.0545/kWh
	Cooling Water	\$3.85/100 gallons
<i>Total Utility Cost/year</i>		\$2,200,000
Water Treatment		\$0.0006/lb
<i>Total Water Treatment Cost/year</i>		\$5,600
Operating Labor		\$410,000
Direct Supervisory and Clerical Labor		\$74,000
Maintenance and Repairs		\$643,000
Operating Supplies		\$97,000
Laboratory Charges		\$62,000
<i>Total Direct Manufacturing Costs</i>		\$58,720,000
Local Taxes and Insurance		\$343,000
Plant Overhead Costs		\$676,000
<i>Total Fixed Manufacturing Costs</i>		\$1,020,000
Total Cost of Production Cost		\$59,800,000
Cost of Nylon-6,6		\$1.04/lb

The details of the utility requirements for this process are summarized in Table 15, below.

Table 15: Summary of Annual Utility Costs

Utility Stream	Cost/year
Mixer Heating	\$387,000
Mixer Mixing	\$291,000
Reactor Heating	\$383,000
Reactor Mixing	\$287,000
Feed Water Pump	\$3
Extruder	\$1,540,000
Cooling Water Cost	\$350,000
Total Cost of Utilities	\$3,230,000

The working capital for this design is the raw materials present in storage tanks before being introduced to the process. There are two storage tanks for each reactant and each tank has the capability to hold two days' worth of material. In total, there is four days' worth of each reactant on site that is treated as working capital. The maximum amount of working capital in the facility at any given time is summarized in the table below.

Table 16: Working Capital Summary

Material	Working Capital
Adipic Acid	\$409,049
HMDA	\$595,267
Water	\$3
Total	\$1,004,318

The total capital investment is \$10,800,000. As mentioned previously in this report, the detailed costing equations for each piece of equipment can be seen on pages 57 and 58 in the Appendix.

Economic Analysis

The profitability of this design was assessed by calculating the discounted cash flow rate of return (DCFROR) and the net present value (NPV). A minimum rate of return of 15% was assumed. These factors were calculated over a fifteen year span, accounting for ten year MACRS depreciation of capital. It was assumed that 60% of the fixed capital investment was incurred in 2018 and the remaining 40% was incurred in 2019. The recommended start up is July 2019, and half year production was assumed for that

year. The payback period was calculated to determine the length of time to recover the costs of investment. The same economic factors were considered when evaluating operation at 67% capacity. A summary of the results of the profitability indicators for 100% capacity operation and 67% capacity operation is seen below in Table 17 and Table 18, respectively.

Table 17: 100% Capacity

DCFROR	113%
NPV	\$69,300,000
Payback Period	0.88 years

Table 18: 67% Capacity

DCFROR	70%
NPV	\$33,500,000
Payback Period	1.34 years

The cash flow sheets for operating at 100% capacity and 67% capacity are included on the next two pages, respectively.

Production of Nylon-6,6
 Corporate Financial Situation
 Minimum ROR
 other

i* 0.15

	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032
Year	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Production (Nylon-6,6) (lb)			42500000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000
Sales Price (Nylon-6,6) (\$/lb)			\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36
Sales Revenue	0	0	57,800,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000
Net Revenue	0	0	57,800,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000	115,600,000
Manufacturing Costs (\$)			(44,010,290)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)	(88,020,580)
Depreciation (60%)			(642,580)	(1,156,644)	(925,315)	(740,252)	(592,459)	(473,581)	(420,890)	(420,890)	(421,532)	(420,890)	(210,766)			
Depreciation (40%)				(428,386)	(771,096)	(616,877)	(493,501)	(394,972)	(315,721)	(280,593)	(280,593)	(281,022)	(280,593)	(140,511)		
Loss Forward																
Writeoff (60%)																
Writeoff (40%)																
Taxable income	0	0	13,147,130	25,994,390	25,883,010	26,222,292	26,493,461	26,710,867	26,842,810	26,877,938	26,877,295	26,877,509	27,088,061	27,438,910	27,579,420	27,579,420
Tax @ 40%	0	0	(5,258,852)	(10,397,756)	(10,353,204)	(10,488,917)	(10,597,384)	(10,684,347)	(10,737,124)	(10,751,175)	(10,750,918)	(10,751,004)	(10,835,224)	(10,975,564)	(11,031,768)	(11,031,768)
Net Income	0	0	7,888,278	15,596,634	15,529,806	15,733,375	15,896,076	16,026,520	16,105,686	16,126,763	16,126,377	16,126,505	16,252,837	16,463,346	16,547,652	16,547,652
Depreciation (60%)			642,580	1,156,644	925,315	740,252	592,459	473,581	420,890	420,890	421,532	420,890	210,766	0	0	0
Depreciation (40%)				428,386	771,096	616,877	493,501	394,972	315,721	280,593	280,593	281,022	280,593	140,511	0	0
Loss Forward																
Writeoff											0			0		
Working Capital																
Fixed Capital		(6,425,797)	(4,283,865)													
Cash Flow	0	(6,425,797)	4,246,993.045	17,181,664	17,226,216	17,090,504	16,982,036	16,895,074	16,842,296	16,828,245	16,828,502	16,828,417	16,744,196	16,603,857	16,547,652	16,547,652
Discount Factor	1.0000	0.9286	0.7993	0.6879	0.5921	0.5096	0.4387	0.3776	0.3250	0.2797	0.2407	0.2072	0.1783	0.1535	0.1321	0.1137
Discounted Cash Flow	0	(5,967,060)	3,394,494	11,819,782	10,199,815	8,709,833	7,449,170	6,378,735	5,473,073	4,706,692	4,051,125	3,486,848	2,986,160	2,548,692	2,186,276	1,881,634
NPV @i*		69,305,270														
DCFROR		112.9169														

FCI
 \$10,709,662

60% of FCI incurred in 2018
 40% occurred in 2019
 Startup in July 2019
 Half Year of Production in 2019

Figure 16: Cash Flow Sheet: 100% Capacity

Production of Nylon-6,6
 Corporate Financial Situation
 Minimum ROR
 other
 i*

0.15

	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032
Year	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Production (Nylon-6,6) (lb)			42500000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000
Capacity Factor			0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67
Sales Price (Nylon-6,6) (\$/lb)			\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36	\$1.36
Sales Revenue	0	0	38,726,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000
Net Revenue	0	0	38,726,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000	77,452,000
Manufacturing Costs (\$)			(29,866,710)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)	(59,733,420)
Depreciation (60%)			(642,580)	(1,156,644)	(925,315)	(740,252)	(592,459)	(473,581)	(420,890)	(420,890)	(421,532)	(420,890)	(210,766)			
Depreciation (40%)				(428,386)	(771,096)	(616,877)	(493,501)	(394,972)	(315,721)	(280,593)	(280,593)	(281,022)	(280,593)	(140,511)		
Loss Forward																
Writeoff (60%)																
Writeoff (40%)																
Taxable income	0	0	8,216,710	16,133,550	16,022,169	16,361,451	16,632,620	16,850,026	16,981,969	17,017,097	17,016,454	17,016,669	17,227,220	17,578,069	17,718,580	17,718,580
Tax @ 40%	0	0	(3,286,684)	(6,453,420)	(6,408,868)	(6,544,581)	(6,653,048)	(6,740,010)	(6,792,788)	(6,806,839)	(6,806,582)	(6,806,667)	(6,890,888)	(7,031,228)	(7,087,432)	(7,087,432)
Net Income	0	0	4,930,026	9,680,130	9,613,302	9,816,871	9,979,572	10,110,016	10,189,182	10,210,258	10,209,873	10,210,001	10,336,332	10,546,841	10,631,148	10,631,148
Depreciation (60%)			642,580	1,156,644	925,315	740,252	592,459	473,581	420,890	420,890	421,532	420,890	210,766	0	0	0
Depreciation (40%)				428,386	771,096	616,877	493,501	394,972	315,721	280,593	280,593	281,022	280,593	140,511	0	0
Loss Forward																
Writeoff											0			0		
Working Capital																
Fixed Capital		(6,425,797)	(4,283,865)													
Cash Flow	0	(6,425,797)	1,288,741	11,265,160	11,309,712	11,173,999	11,065,532	10,978,569	10,925,792	10,911,741	10,911,998	10,911,912	10,827,692	10,687,352	10,631,148	10,631,148
Discount Factor	1.0000	0.9286	0.7993	0.6879	0.5921	0.5096	0.4387	0.3776	0.3250	0.2797	0.2407	0.2072	0.1783	0.1535	0.1321	0.1137
Discounted Cash Flow	0	(5,967,060)	1,030,052	7,749,641	6,696,594	5,694,605	4,853,896	4,144,959	3,550,445	3,051,905	2,626,845	2,260,948	1,931,011	1,640,509	1,404,587	1,208,868
NPV @i*																
DCFROR																

60% of FCI incurred in 2018
 40% occurred in 2019
 Startup in July 2019
 Half Year of Production in 2019

FCI
 \$10,709,662

Figure 17: Cash Flow Sheet: 67% Capacity

A sensitivity analysis was performed to identify the parameters that have the largest impact on the profitability of the design. The following parameters were included in the analysis: selling price of Nylon-6,6, purchase of cost of Adipic Acid, purchase cost of HMDA, cost of water treatment, capital cost, and cost of utilities. The parameters that have the greatest effect on the profitability of the design are selling price of Nylon-6,6 and purchase cost of Adipic Acid and HMDA. The following tables show the detailed sensitivity analysis on these parameters.

Table 19: Sensitivity Analysis for Selling Price of Nylon-6,6

Market Price (\$/lb N66)	Change in Prediction	ROR%	% Change in ROR	NPV
\$1.04	-24%	-18.9	-116.7	(6,350,253)
\$1.20	-12%	54.14	-52.1	\$31,477,508
\$1.36	0	112.92	0.0	\$69,305,270
\$1.52	12%	170.19	50.7	\$107,133,029
\$1.77	30%	258.27	128.7	\$166,238,905
\$2.00	47.10%	338.48	199.8	\$220,616,312

The price range used in this sensitivity analysis was selected because of historic market trends. The lowest selling price corresponds to the cost of production/lb of Nylon-6,6. If the market selling price were to fall below \$1.04/lb of Nylon-6,6, it would not be feasible to continue operation with the current design. The break-even price is \$1.07/lb of Nylon-6,6.

Table 20: Sensitivity Analysis for Purchase Price of Adipic Acid

Cost of Adipic Acid (\$/lb ADIPIC ACID)	Change in Prediction	ROR%	% Change in ROR	NPV
\$0.34	-45%	175.74	55.6	\$110,833,172
\$0.43	-30%	155.08	37.3	\$97,092,322
\$0.52	-15%	134.3	18.9	\$83,351,472
\$0.61	0	112.92	0.0	\$69,305,270
\$0.70	15%	92.28	-18.3	\$55,869,772
\$0.79	30%	70.93	-37.2	\$42,128,922
\$0.88	45%	49.21	-56.4	\$28,388,072

Table 21: Sensitivity Analysis for Purchase Price of HMDA

Cost of HMDA (\$/lb HMDA)	Change in Prediction	ROR%	% Change in ROR	NPV
\$0.62	-45%	204.89	81.4	\$130,313,870
\$0.78	-30%	175.83	55.7	\$110,888,830
\$0.95	-15%	114.75	1.6	\$90,249,726
\$1.12	0	112.92	0.0	\$69,305,270
\$1.29	15%	81.6	-27.7	\$48,971,517
\$1.46	30%	49.12	-56.5	\$28,332,413
\$1.62	45%	16.98	-85.0	\$8,907,374

The price range for cost of Adipic Acid and cost of HMDA was determined so as to reflect changing market trends.

The tornado chart on the following page represents the effect of each parameter on the rate of return. The cost of water treatment has such a small effect on the economic analysis that it is not included on the tornado chart.

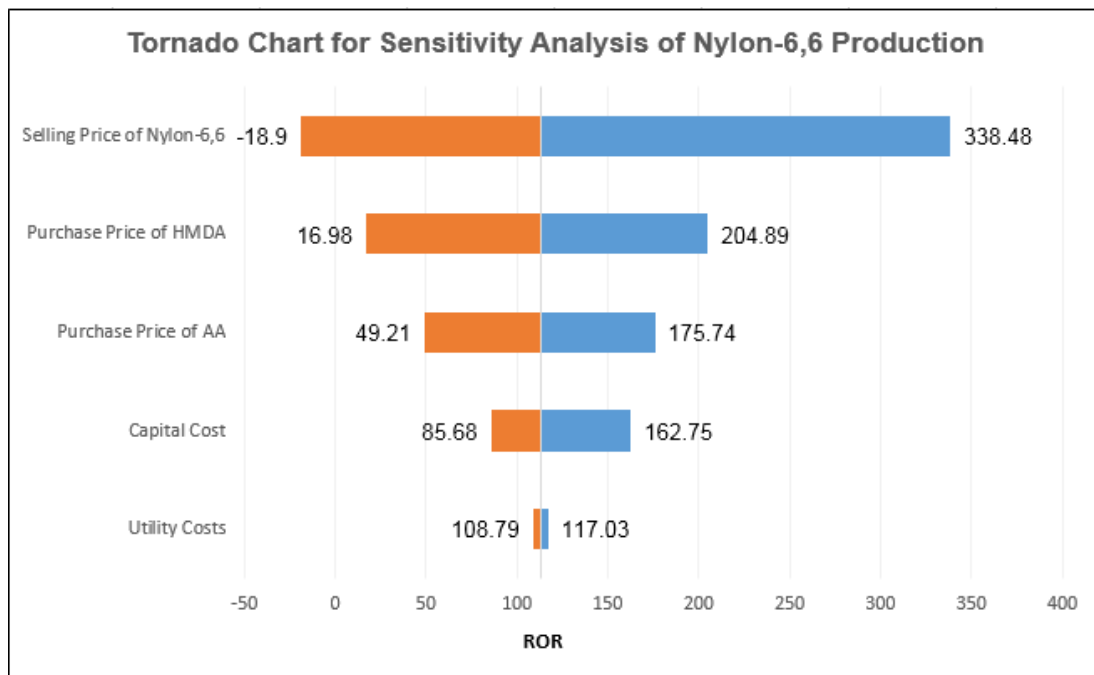


Figure 18: Tornado Chart for Sensitivity Analysis

Based on the results from the sensitivity analysis, a best case and worst case scenario were developed. This provides perspective on the potential of the project on both ends of the spectrum. The best case scenario considers the highest selling price of Nylon-6,6 and the lowest costs of raw materials, water treatment, and capital and operating expenses. The worst case scenario considers the lowest selling price of Nylon-6,6 and the highest costs of raw materials, water treatment, and capital and operating expenses. The results from this analysis are summarized below in Table 22. Cash flow sheets for the best case and the worst case are found on pages 79 and 80 in the Appendix, respectively.

Table 22: Best Case/Worst Case Scenarios

	Worst Case	Best Case
Market Price (\$/N66)	\$1.04	\$2.00
Cost of Adipic Acid (\$/lb)	\$0.88	\$0.34
Cost of HMDA (\$/LB)	\$1.62	\$0.62
Cost of Water Treatment (\$/lb)	\$0.00105	\$0.00015
Capital Cost	\$13,922,561	\$7,496,764
Utility Cost (\$/year)	\$4,197,358	\$2,260,116
NPV	(112,296,223)	328,388,211
ROR	>>0%	701%

The results of the economic analysis indicate that this design, at 100% capacity and 67% capacity, is profitable and should progress to the detailed design phase. The calculated DCFROR exceeds the minimum rate of return and the NPV is positive, indicating profitability. The payback period does not exceed two years for either case, which indicates the capital investment will be recovered within a reasonable amount of time. The combination of these economic indicators leads the design team to recommend moving forward to detailed design stage.

Conclusions and Recommendations

It is recommended that this process moves to the detailed design phase. The design team recommends implementing the safety procedures outlined in this report to ensure safe operation. It is advised to implement a batch process that consists of four cycles per day and utilizes four mixers and four reactors. A fifth mixer and reactor should be purchased and used in rotation to allow for cleaning of the vessels every eight days. The recommended volume of each mixer is 452 ft³ and the recommended volume for each reactor is 481 ft³.

The design team concludes that the production process of Nylon-6,6 from Adipic Acid and HMDA is feasible and profitable. The safety and environmental effects of this design were critical considerations when determining feasibility. After thorough analysis, the team mitigated potential risks to health and the environment. This design requires a fixed capital investment of \$10,800,000. Ten year depreciation of equipment was assumed. The economic analysis indicates profitability with a NPV of \$69,300,000 and rate of return of 113%, when analyzed over a fifteen year span. Detailed analysis of this process should begin as soon as possible to capitalize on the opportunity in the market.

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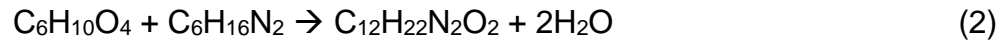
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Appendix

Equations

Reaction Information



$$-rA = kC_{\text{Adipic Acid}}C_{\text{HMDA}} \quad (3)$$

Where:

rA = reaction rate, (mol/L*hour)

k = rate constant, (1/hour)

$C_{\text{Adipic Acid}}$ = concentration of Adipic Acid (mol/L)

C_{HMDA} = concentration of HMDA (mol/L)

$$\frac{dX}{dt} = \frac{rAV_{\text{reactor}}}{N_{a0}} \quad (4)$$

Where:

X = conversion to Nylon-6,6

t = time (hours)

rA = reaction rate, (mol/L*hour)

V_{reactor} = volume of the reactor (ft³)

N_{a0} = initial moles of Adipic Acid (moles)

Material Balance

$$\left(85 \times 10^6 \frac{\text{lb}}{\text{year}} \text{N66}\right) * \left(\frac{1 \text{ mol AA}}{1 \text{ mol N66}}\right) \left(\frac{146.14 \frac{\text{g}}{\text{mol}}}{226.304 \frac{\text{g}}{\text{mol}}}\right) = 54.88 \times 10^6 \frac{\text{lb}}{\text{year}} \text{AA} \quad (5)$$

$$\left(85 \times 10^6 \frac{\text{lb}}{\text{year}} \text{N66}\right) * \left(\frac{1 \text{ mol HMDA}}{1 \text{ mol N66}}\right) \left(\frac{116.21 \frac{\text{g}}{\text{mol}}}{226.304 \frac{\text{g}}{\text{mol}}}\right) = 43.65 \times 10^6 \frac{\text{lb}}{\text{year}} \text{HMDA} \quad (6)$$

$$\left(85 \times 10^6 \frac{\text{lb}}{\text{year}} \text{N66}\right) * \left(\frac{2 \text{ mol H}_2\text{O}}{1 \text{ mol N66}}\right) * \left(\frac{18.051 \frac{\text{g}}{\text{mol}}}{226.304 \frac{\text{g}}{\text{mol}}}\right) = 13.56 \times 10^6 \frac{\text{lb}}{\text{year}} \text{H}_2\text{O} \quad (7)$$

Energy Balance

Mixer

$$\dot{Q}_{mixer} = \dot{m}_{mixture} C_{p,mixture} (T_{exit,m} - T_{inlet,m}) \quad (8)$$

Where:

\dot{Q}_{mixer} = heat flow from the mixer, (Btu/hour)

$\dot{m}_{mixture}$ = mass flow rate of water, Adipic Acid, and HMDA to the mixer (lb/day)

$C_{p, mixture}$ = heat capacity of water, Adipic Acid, and HMDA mixture (Btu/°F)

$T_{exit,m}$ = exit temperature of the mixer, (°F)

$T_{inlet,m}$ = inlet temperature of the mixer, (°F)

Polymerization Reactor

$$\dot{Q}_{reactor} = \dot{m}_{solution} C_{p,solution} (T_{exit,r} - T_{inlet,r}) + \Delta H_{rxn} \quad (9)$$

Where:

$\dot{Q}_{reactor}$ = heat flow from the reactor, (Btu/hour)

$\dot{m}_{solution}$ = mass flow rate of water, Adipic Acid, and HMDA solution to the reactor (lb/day)

$C_{p, solution}$ = heat capacity of water, Adipic Acid, and HMDA solution (Btu/°F)

$T_{exit,r}$ = exit temperature of the reactor, (°F)

$T_{inlet,r}$ = inlet temperature of the reactor, (°F)

ΔH_{rxn} = heat of reaction of Adipic Acid and HMDA to form Nylon-6,6 and water (Btu/lb)

Cooling the Product

$$\dot{Q}_{Cooled Product} = \dot{m}_{N66} C_{p,N66} (T_{final,N66} - T_{initial,N66}) \quad (10)$$

Where:

$\dot{Q}_{Cooled Product}$ = heat released through cooling process, (Btu/hour)

\dot{m}_{N66} = mass flow rate of molten Nylon-6,6 (lb/day)

$C_{p, N66}$ = heat capacity of molten Nylon-6,6 (Btu/°F)

$T_{final,N66}$ = final temperature of Nylon-6,6 product, (°F)

$T_{initial,N66}$ = initial temperature of Nylon-6,6 product, (°F)

Required Water to Completely Dissolve Reactants

$$F_{water} = F_{Adipic\ Acid} \frac{x_{Water}}{x_{Adipic\ Acid}} \quad (11)$$

Where:

F_{water} = molar flow rate of water, (mol/day)

$F_{Adipic\ Acid}$ = molar flow of Adipic Acid, (mol/day)

x_{water} = mole fraction of water

$x_{Adipic\ Acid}$ = mole fraction of Adipic Acid

Water to Pressurize the Mixer

$$n_{water} = \frac{P_{mixer}V_{mixer}}{RT_{mixer}} \quad (12)$$

Where:

n_{water} = moles of water required to pressurize the mixer, (lbmol/mixer)

P_{mixer} = final pressure of the mixer, (psi)

V_{mixer} = volume of one mixer, (ft³)

R = ideal gas constant, (psi*ft³/lbmol*R)

T_{mixer} = temperature in the mixer, (R)

Sizing the Feed Pump

$$BHP = \frac{GPM\Delta P}{7115\eta} \quad (13)$$

BHP = required brake horsepower for the feed pump, (hp)

GPM = flow rate through the pump (GPM)

ΔP = pressure drop across the pump, (psi)

η = efficiency of the pump

Equipment Cost Estimation

Calculating Purchase Cost

$$C_P = C_P^0 F_P F_M \quad (14)$$

Where:

C_P = Purchase cost of equipment

C_P^0 = Purchase cost for base conditions

F_P = Pressure factor

F_M = Material factor, according to Reference 34

Calculating Purchase Cost for Base Conditions

$$\log_{10} C_P^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2 \quad (15)$$

Where:

A = Capacity or size parameter for that equipment

K_1, K_2, K_3 = Correlation coefficients, according to Reference 34

Calculating Pressure Factor

I. Process Vessels

$$F_{P,vessel} = \frac{\frac{(P+1)D}{2[850-0.6(P+1)]} + 0.00315}{0.0063} \quad (16)$$

Where:

P = pressure of process vessel, (barg)

D = diameter of process vessel, (m)

II. Other Process Equipment

$$\log_{10} F_P = C_1 + C_2 \log_{10} P + C_3 (\log_{10} P)^2 \quad (17)$$

Where:

C_1, C_2, C_3 = correlation coefficients, according to Reference 34

Bare Module Cost

$$C_{BM} = C_P^o F_{BM} = C_P^o (B_1 + B_2 F_M F_P) \quad (18)$$

Where:

C_{BM} = Bare Module Cost

C_P^o = Purchase cost for base conditions

F_{BM} = Bare Module Factor

B_1 = Bare Module Constant

B_2 = Bare Module Constant

F_M = Material Factor

F_P = Pressure Factor

Grassroots Cost

$$C_{TM} = \sum_{i=1}^n C_{TM,i} = 1.18 \sum_{i=1}^n C_{BM,i} \quad (19)$$

$$C_{GR} = C_{TM} + 0.5 \sum_{i=1}^n C_{BM,i}^o \quad (20)$$

Where:

C_{TM} = Total Module Cost

C_{BM} = Bare Module Cost

C_{GR} = Grassroots Cost

Effect of Time of Equipment Cost Calculation

$$C_2 = C_1 \frac{I_2}{I_1} \quad (21)$$

Where:

C_1 = cost in base year

C_2 = cost in desired year

I_1 = cost index in base year

I_2 = cost index in desired year

Utility Cost Estimation

Electricity for Pumps

$$Cost_{pump\ utility} = qhc_{electricity} \quad (22)$$

Where:

Cost_{pump utility} = yearly operating cost of using electricity in a pump

q = heat flow, kW

h = operating hours of the pump per year

C_{electricity} = cost of electricity, (\$/kW hour)

Cooling Water Utility

$$Cost_{Cooling\ Water} = qhc_{Cooling\ Water} \quad (23)$$

Where:

Cost_{Cooling Water} = yearly operating cost of cooling water

q = heat flow, (kW)

h = operating hours of the pump per year

C_{Cooling Water} = cost of cooling water, (\$/lb)

Operating Labor Cost Estimation

$$N_{np} = \sum Equipment \quad (24)$$

Where:

N_{np} = number of nonparticulate processing steps

Equipment = summation of total compressors, exchangers, furnaces, reactors, and towers in process

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \quad (25)$$

Where:

N_{OL} = number of operators per shift

P = number of processing steps involving the handling of particulate solids

$$Labor\ Costs = 4.5N_{OL}W \quad (25)$$

Where:

Labor Costs = cost of labor to run this unit for one year

W = annual wage of operators

NPV Calculation

$$NPV = \sum_{i=1}^n \text{Cash flow} \frac{P}{F_{i,n}} \quad (27)$$

Where:

NPV = net present value

Cash flow = after tax cash flow per year

$\frac{P}{F_{i,n}}$ = discount factor

Table 23: Energy Balance around Reactors and Mixers

	Total/Day	2 Cycles	3 Cycles	4 Cycles		
Hours in Cycle	24	12	8	6	Mixer	
Q _{mixer} , (Btu/h)	2611534	2611534	2611534	2611534		
Q (Btu/cycle)	62676827	31338413	20892276	15669207		
Mass of Water (lb/day)	1277.00	638.50	425.67	319.25		
Mass of HMDA	132872.00	66436.00	44290.67	33218.00		
Mass of AA	167095.00	83547.50	55698.33	41773.75		
C _p , mixture	1.01	1.01	1.01	1.01		
T, initial (F)	60	60	60	60		
T, final (F)	266	266	266	266		
Q _{polyreactor} (Btu/h)	2580420	2580420	2580420	2580420	Reactor	
Q (Btu/cycle)	61930079	30965040	20643360	15482520		
H _{vap} , water (Btu/lb)	970	970	970	970		
Mass of water	41278.00	20639.00	13759.33	10319.50		
Q, water (Btu)	1668319	1668319	1668319	1668319		
Q, nylon	911971	911971	911971	911971		
Mass of Nylon (lb)	258752.00	129376.00	86250.67	64688.00		
C _p , Nylon	0.399	0.399	0.399	0.399		
T, initial, Nylon	266	266	266	266		
T, final, Nylon	478	478	478	478		
deltaH, rxn (Btu/lb)	0.012	0.012	0.012	0.012		
Q, rxn	129.376	129.376	129.376	129.376		
Mass of AA	167095.00	83547.50	55698.33	41773.75		Reactants
Moles of AA	1143.40	571.70	381.13	285.85		
Volume of AA		0.00	0.00	0.00		
Mass of HMDA	132872.00	66436.00	44290.67	33218.00		
Moles of HMDA	1143.40	571.70	381.13	285.85		
Volume of HMDA		0.00	0.00	0.00		
Mass of Water	1277.00	638.50	425.67	319.25		
Moles of Water	70.94	35.47	23.65	17.74		
Volume of Water		0.00	0.00	0.00		
Mass of Nylon 66	258752.00	129376.00	86250.67	64688.00	Products	
Moles of Nylon 66	1143.40	571.70	381.13	285.85		
Volume of Nylon 66		0.00	0.00	0.00		
Mass of Prod Water	41278.00	20639.00	13759.33	10319.50		
Moles of Prod Water	2286.80	1143.40	762.27	571.70		
Volume of Prod Water		0.00	0.00	0.00		

Table 24: Electricity Costs for Mixers and Reactors

Heating Cost of Mixer	
Qm (Btu/hr)	2611534
Efficiency	0.85
Qm (kWhr)	900.4670172
Cost/day	\$1,177.81
Cost/year	\$386,910.87

-includes ServF

Agitator Cost of Mixer	
Qm (Btu/hr)	1958650
Efficiency	0.85
Qm (kWhr)	675.35
Cost/day	\$883.36
Cost/year	\$290,183.00

-includes ServF

Heating Cost of PR	
Qpr (Btu/hr)	2580420
Efficiency	0.85
Qpr (kWhr)	889.7386272
Cost/day	\$1,163.78
Cost/year	\$382,301.11

-includes ServF

Agitator Cost of PR	
Qpr (Btu/hr)	1935316
Efficiency	0.85
Qpr (kWhr)	667.30
Cost/day	\$872.83
Cost/year	\$286,726.00

-includes ServF

Table 25: Optimization of Purchase Water Cost vs. Operating Costs

Water Inlet Temp (F)		60		Heating Efficiency		0.8					
Temp (K)	Temp (F)	Cp,water(T) (Btu/lb/F)	Duty Required (Btu/h)	Duty Required (kW)	Operating Cost (\$/day)	Volume Water (L/day)	Density (lb/ft3)	Density (lb/L)	Mass Water (lb/h)	Water Purchase Cost/Day	Total Cost (\$/yr)
303	86	1	16109.25	4.72	\$6.18	5,416	62.16	2.20	495.67	\$7.14	\$4,373.37
313	104	1	18576.38	5.44	\$7.12	3,706	61.90	2.19	337.75	\$4.86	\$3,937.05
323	122	1	18051.25	5.29	\$6.92	2,564	61.70	2.18	232.92	\$3.35	\$3,375.02
333	140	1	14870.88	4.36	\$5.70	1,645	61.40	2.17	148.71	\$2.14	\$2,576.16
343	158	1	13268.31	3.89	\$5.09	1,206	61.00	2.16	108.31	\$1.56	\$2,183.26
353	176	1	12070.48	3.54	\$4.63	933	60.60	2.14	83.24	\$1.20	\$1,913.83
363	194	1.01	11760.28	3.45	\$4.51	783	60.30	2.13	69.52	\$1.00	\$1,809.82
373	212	1.01	11778.33	3.45	\$4.52	697	59.81	2.11	61.38	\$0.88	\$1,773.60
383	230	1.01	11655.41	3.42	\$4.47	622	59.30	2.10	54.31	\$0.78	\$1,724.67
393	248	1.01	11712.34	3.43	\$4.49	570	58.80	2.08	49.35	\$0.71	\$1,708.38
403	266	1.02	11635.72	3.41	\$4.46	517	58.20	2.06	44.30	\$0.64	\$1,674.87

*This calculation does not include the amount of water added to pressurize the mixer or the amount of HMDA or AA heated, but as these values are nearly constant, this cost comparison is not impacted.

Table 26: Amount of Water to Be Evaporated

Initial	Wt. Water	42668
	Wt. Dry Material	258752
	% Water	14.16%
Final	Wt. Water	517.504
	Wt. Dry Material	258752
	% Water	0.20%
Lb water Evap	42150.496	

Table 27: Heat Exchanger Sizing for Condensing Steam

Condenser		
CW Temp Cold	60	F
CW Temp Hot	100	F
Nylon-6,6 Temp Cold	194	F
Nylon-6,6 Temp Hot	494.5	F
delta T log mean	241.25	
U	150	Btu/hr*ft2*F
R	0.2650	
P	0.3400	
F	1	
Q	131380000	Btu/hr
A	3630.49	ft2

mdot CW	3284500	lb/h
Cp CW (87deg)	1	Btu/lb*F
deltaT CW	40	F

Cost of CW	0.000106	\$/lb
Operating Cost (\$/year)	\$2,744,870	(\$/year)

Table 28: Determining Reaction Constant, K

T (K)	k (1/sec)	Time (sec)	Time (hr)	N66 (lbmol/hr)	N66 (lbm/hr)	k (1/hr)
520	0.00071250	4352	1.208889	40.7113	9200.7538	2.564990416
521	0.00068473	4703.5	1.306528	40.7078	9199.9628	2.465023377
522	0.00065814	5091.4	1.414278	40.7093	9200.3018	2.369313265
523	0.00063268	5502.5	1.528472	40.7083	9200.0758	2.277664215
524	0.00060830	5958	1.655000	40.7169	9202.0194	2.189890016
525	0.00058495	6433.8	1.787167	40.7081	9200.0306	2.105813604
526	0.00056257	6949.5	1.930417	40.7116	9200.8216	2.02526659
527	0.00054114	7514.3	2.087306	40.7076	9199.9176	1.948088801
528	0.00052059	8095.5	2.248750	40.7101	9200.4826	1.874127854
529	0.00050090	8760.7	2.433528	40.7096	9200.3696	1.803238758
530	0.00048202	9459.1	2.627528	40.7079	9199.9854	1.735283525
531	0.00046393	10207	2.835278	40.7075	9199.895	1.670130815
532	0.00044657	11004	3.056667	40.7087	9200.1662	1.607655594
533	0.00042993	11881	3.300278	40.7111	9200.7086	1.547738807
534	0.00041396	12813	3.559167	40.708	9200.008	1.490267081
535	0.00039865	13806	3.835000	40.7152	9201.6352	1.43513243
536	0.00038395	14888	4.135556	40.7089	9200.2114	1.382231986
537	0.00036985	16036	4.454444	40.7076	9199.9176	1.331467738
538	0.00035632	8542.3	2.372861	40.7092	9200.2792	1.282746289

Table 29: Temperature Effects on Solubility

Inlet Temp (K)	Solubility of AA (xi)	Mole Fraction of Water	Molar Flow of Water (mol/day)	Mass Flow of Water (g/day)	Mass Flow of Water (lb/day)	Volume Flow of Water (L/day)	Cost of Water (\$/hr)
303	0.004	0.996	284,607	5,122,926	11,296	5,145	\$67.91
313	0.006	0.994	189,357	3,408,426	7,516	3,435	\$45.34
323	0.009	0.991	125,857	2,265,426	4,995	2,293	\$30.27
333	0.015	0.985	75,057	1,351,026	2,979	1,374	\$18.14
343	0.022	0.978	50,812	914,608	2,017	935	\$12.34
353	0.031	0.969	35,728	643,103	1,418	662	\$8.73
363	0.04	0.96	27,432	493,776	1,089	512	\$6.75
373	0.048	0.952	22,670	408,051	900	426	\$5.62
383	0.058	0.942	18,564	334,150	737	351	\$4.64
393	0.068	0.932	15,666	281,985	622	299	\$3.95
403	0.082	0.918	12,796	230,328	508	246	\$3.25

Table 30: Calculating Volume of Dissolving Water

Solubility of HMDA (g/L)	490
Molar Flow of HMDA (mol/day)	1143
MW of HMDA (g/mol)	116.21
Mass Flow of HMDA (g/day)	132828.03
Volume Flow of Water (L/day)	271.0776122
Mass Flow of Water (lb/day)	595.1559126

Inlet Temperature (K)	Total Volume of Water Needed (L/day)	Total Mass Flow of Water (lb/day)	Mass Flow Rate (lb/hr)
303	5,416	11891.20774	495.4669893
313	3705.952146	8110.735243	337.9473018
323	2564.018908	5590.420243	232.9341768
333	1645.468253	3574.168243	148.9236768
343	1206.25943	2611.866152	108.8277563
353	932.7066445	2013.198952	83.88328968
363	782.7625863	1683.931993	70.16383303
373	697.0181133	1494.908368	62.28784865
383	622.4447394	1,332	55.49820695
393	570.1071176	1,217	50.70551869
403	517.4181887	1,103	45.95958836

Table 31: Optimizing Cycles per Day and Number of Reactors Per Day

4 Cycles/Day	
Volume m3	42.70

3 Cycles/Day	
Volume m3	56.93

2 Cycles/Day	
Volume m3	85.40

# of Reactors	MV m3	Cost/Reactor	Total Cost	# of Reactors	MV m3	Cost/Reactor	Total Cost	# of Reactors	MV m3	Cost/Reactor	Total Cost
1	42.700	\$510,088.66	\$510,088.66	1	56.934	\$594,157.48	\$594,157.48	1	85.400	\$736,643.75	\$736,643.75
2	21.350	\$353,136.99	\$706,273.98	2	28.467	\$411,373.89	\$822,747.77	2	42.700	\$510,088.66	\$1,020,177.32
3	14.233	\$284,761.49	\$854,284.46	3	18.978	\$331,739.18	\$995,217.53	3	28.467	\$411,373.89	\$1,234,121.66
4	10.675	\$244,427.54	\$977,710.15	4	14.233	\$284,761.49	\$1,139,045.95	4	21.350	\$353,136.99	\$1,412,547.96
5	8.540	\$217,114.57	\$1,085,572.85	5	11.387	\$252,948.55	\$1,264,742.76	5	17.080	\$313,697.62	\$1,568,488.08
6	7.117	\$197,076.65	\$1,182,459.88	6	9.489	\$229,608.67	\$1,377,652.03	6	14.233	\$284,761.49	\$1,708,568.92
8	5.338	\$169,147.83	\$1,353,182.65	8	7.117	\$197,076.65	\$1,576,613.18	8	10.675	\$244,427.54	\$1,955,420.30
10	4.270	\$150,236.72	\$1,502,367.22	10	5.693	\$175,047.91	\$1,750,479.13	10	8.540	\$217,114.57	\$2,171,145.70
15	2.847	\$121,113.08	\$1,816,696.24	15	3.796	\$141,121.73	\$2,116,825.97	15	5.693	\$175,047.91	\$2,625,718.69
20	2.135	\$103,937.58	\$2,078,751.64	20	2.847	\$121,113.08	\$2,422,261.65	20	4.270	\$150,236.72	\$3,004,734.43

Table 32: Determining Mixer Volume

Mass of Water (lb/day)	1277
Density of Water (lb/L)	2.204
Volume of Water (L/day)	579
Volume HMDA (L/day)	71823
Volume AA (L/day)	55698
Total Volume (L/day)	128100
Safety Factor	0.75
Adjusted Volume (L)	170800.5348
Adjusted Volume (m3)	170.8005348

Table 33: Determining Water Required to Pressurize Mixer

Dissolving Water	517	L/day
	2.205	lb/L
	1139.99	lb/day
Water to Pressurize	0.8681	lbmol/mixer
(PV/RT)	250.04	lb/day
Total Water Needed	1390	lb/day
V	169	ft3/mixer
R	10.731	psi-ft3/R-lbmol
P	40	psi
T	725.67	R

Table 34: Overall Mass Balance

Molecular Wt. (lb/lbmol)	146.1412	226.304	18.051	
	HMDA	Adipic Acid	Nylon 66	Water
Per Year (lb)	0	54890775	85000000	13559946
Per Day (lb)	0	167095	258752	41278
Service Factor	0.9	Safety Factor	0.75	

Table 35: Optimizing Number of Reactors

4 Cycles/Day	
Mass of Water (lb)	10319.59
Density of Water (lb/ft3)	62.40
Volume of Water (ft3)	165.38
Mass of Nylon (lb)	64687.98
Density of Nylon (lb/ft3)	56.12
Volume of Nylon (ft3)	1152.67
Total Volume (ft3)	1318.05
Adjusted Volume (ft3)	1757.40

3 Cycles/Day	
Mass of Water (lb)	13759.46
Density of Water (lb/ft3)	62.40
Volume of Water (ft3)	220.50
Mass of Nylon (lb)	86250.63
Density of Nylon (lb/ft3)	56.12
Volume of Nylon (ft3)	1536.90
Total Volume (ft3)	1757.40
Adjusted Volume (ft3)	2343.20

2 Cycles/Day	
Mass of Water (lb)	20639.19
Density of Water (lb/ft3)	62.40
Volume of Water (ft3)	330.76
Mass of Nylon (lb)	129375.95
Density of Nylon (lb/ft3)	56.12
Volume of Nylon (ft3)	2305.34
Total Volume (ft3)	2636.10
Adjusted Volume (ft3)	3514.80

# of Reactors	Reactor Vol ft3	RV m3	Cost/Reactor	Total Cost	# of Reactors	Mixer Vol ft3	MV m3	Cost/Reactor	Total Cost	# of Reactors	Mixer Vol ft3	MV m3	Cost/Reactor	Total Cost
1	1757.40	49.764	\$553,229.67	\$553,229.67	1	2343.20	66.352	\$644,396.33	\$644,396.33	1	3514.80	99.528	\$798,908.96	\$798,908.96
2	878.70	24.882	\$383,021.38	\$766,042.77	2	1171.60	33.176	\$446,178.07	\$892,356.15	2	1757.40	49.764	\$553,229.67	\$1,106,459.35
3	585.80	16.588	\$308,867.90	\$926,603.69	3	781.07	22.117	\$359,815.59	\$1,079,446.77	3	1171.60	33.176	\$446,178.07	\$1,338,534.22
4	439.35	12.441	\$265,124.56	\$1,060,498.23	4	585.80	16.588	\$308,867.90	\$1,235,471.59	4	878.70	24.882	\$383,021.38	\$1,532,085.54
5	351.48	9.953	\$235,502.35	\$1,177,511.73	5	468.64	13.270	\$274,365.92	\$1,371,829.58	5	702.96	19.906	\$340,249.48	\$1,701,247.42
6	292.90	8.294	\$213,769.97	\$1,282,619.83	6	390.53	11.059	\$249,052.85	\$1,494,317.09	6	585.80	16.588	\$308,867.90	\$1,853,207.38
8	219.68	6.220	\$183,478.96	\$1,467,831.70	8	292.90	8.294	\$213,769.97	\$1,710,159.77	8	439.35	12.441	\$265,124.56	\$2,120,996.47
10	175.74	4.976	\$162,968.02	\$1,629,680.17	10	234.32	6.635	\$189,878.12	\$1,898,781.16	10	351.48	9.953	\$235,502.35	\$2,355,023.46
15	117.16	3.318	\$131,379.94	\$1,970,699.05	15	156.21	4.423	\$153,081.81	\$2,296,227.11	15	234.32	6.635	\$189,878.12	\$2,848,171.73
20	87.87	2.488	\$112,750.61	\$2,255,012.23	20	117.16	3.318	\$131,379.94	\$2,627,598.73	20	175.74	4.976	\$162,968.02	\$3,259,360.34

Table 36: Pump Sizing

Feed Water Pump		
Suction Pressure	14.7	psi
Discharge Pressure	40	psi
Q	83.32	gpm
hhp	1.23	hp
Pump Efficiency	0.45	Table 11.9
bhp	2.73	hp
bhp, corrected	5	
Motor Efficiency	0.811	Figure 8.7
php	6.17	hp
php	4.60	Kw
Uptime	10.95	h

Required Electricity	50	kW-h
----------------------	----	------

Fill Time	0.5	min
-----------	-----	-----

Electricity Cost (per year)	\$2.74
-----------------------------	--------

Dissolved Salt Pump		
Suction Pressure	40	psi
Discharge Pressure		psi
Q		gpm
hhp	0.00	hp
Pump Efficiency	0.65	Table 11.9
bhp	0.00	hp
bhp, corrected	40	
Motor Efficiency	0.89	Figure 8.7
php	44.94	hp
php	33.51	Kw
Uptime	8322	h

Required Electricity	278909	kW-h
----------------------	--------	------

V (L/day)	128038
Mass (lb/day)	300476.36
Density (lb/L)	2.346774864
Density (lb/ft3)	66.45263666
P (lb/ft2)	265.8105466
Gc	32.174
G	32.174
H (ft)	4
P (psi)	1.845906574

Table 37: CEPCI Values

CEPCI, 2001	397
CEPCI, 2016	540.9

Table 38: Detailed Costing Estimate, Reactant Storage Tanks

AA Storage Tank		Reference	HMDA Storage Tank		Reference
Type	Fixed Roof		Type	Fixed Roof	
log10CPo	4.64313523		log10CPo	4.666266599	
Cpo	\$43,967.85		Cpo	\$46,373.15	
K1	4.8509	A.1	K1	4.8509	A.1
K2	-0.3973		K2	-0.3973	
K3	0.1445		K3	0.1445	
Volume (m3/day)	55.73		Volume (m3/day)	71.8	
How many days?	2		How many days?	2	
Total Volume (m3)	111.46		Total Volume (m3)	143.6	
Fm	3.2	A.3, SS	Fm	3.2	A.3, SS
log10Fp	0.00		log10Fp	0.00	
Fp	1.00		Fp	1.00	
C1	0	A.2	C1	0	A.2
C2	0		C2	0	
C3	0		C3	0	
Pressure (barg)	1.01		Pressure (barg)	1.01	
B1	1.49	A.4	B1	1.49	A.4
B2	1.52		B2	1.52	
CBM	\$279,371.72		CBM	\$294,655.00	
CBM(2016)	\$801,630.04		CBM(2016)	\$401,458.15	
Number of Tanks		2	Number of Tanks		2
Total Cost		\$1,603,260.09	Total Cost		\$802,916.31

Table 39: Detailed Cost Estimate, Conveyor and Extruder

Conveyor		Reference
Type	Belt	
log10CPo	5.2005	
Cpo	\$158,671.89	
K1	4.0637	
K2	0.2584	
K3	0.155	
Area (m2)	100	
FBM	1.25	
CBM	\$198,339.86	
CBM(2016)	\$270,231.82	

Number of Conveyors	1
Total Cost	\$270,231.82

Nylon-6,6 Extruder and Packager		Reference	
Type	Screw Extruder		
log10CPo	4.355305318		
Cpo	\$22,662.37		
K1	3.5565		A.1
K2	0.3776		
K3	0.0905		
Volume (m3)	35		A.3, SS
Fm	3.2		
D (m)	2.00		
Fp	1.06		A.2
C1			
C2			
C3		A.4	
Pressure (barg)	2		
B1	1.49		
B2	2.25		
CBM	\$206,956.69		
CBM(2016)	\$281,971.97		

Additional Cost Factor	2
Total Cost	\$563,943.94

Table 40: Detailed Cost Estimate, Mixer and Reactor

Mixing Reactor		Reference
Type	Jacketed, Agitated	Reactor K-Values Sheet
log10CPo	4.693622747	
Cpo	\$49,388.15	
K1	4.1052	
K2	0.532	
K3	-0.0005	
Volume (m3)	12.8	
FBM	4	
CBM	\$197,552.59	
CBM(2016)	\$269,159.19	

Number of Reactors	5
Total Cost	\$1,345,795.95

Polymerization Reactor		Reference
Type	Jacketed, Agitated	Reactor K-Values Sheet
log10CPo	4.707600244	
Cpo	\$51,003.53	
K1	4.1052	
K2	0.532	
K3	-0.0005	
Volume (m3)	13.6	
FBM	4	
CBM	\$204,014.12	
CBM(2016)	\$277,962.82	

Number of Reactors	5
Total Cost	\$1,389,814.10

Table 41: Detailed Cost Estimate, Water Pump and Storage Tank

Water Feed Pump		Reference
Type	Centrifugal	
log10CPo	3.470073197	
Cpo	\$2,951.71	
K1	3.3892	A.1
K2	0.0536	
K3	0.1538	
Shaft Power (kW)	3.7285	
Fm	1.6	A.3, CS
log10Fp	0.00	
Fp	1.00	
C1	0	
C2	0	A.2
C3	0	
Pressure (barg)	3	
B1	1.89	A.4
B2	1.35	
CBM	\$11,954.41	
CBM(2016)	\$16,287.51	

Number of Pumps	2
Total Cost	\$32,575.02

Feed Water Storage Tank		Reference
Type	Fixed Roof	
log10CPo	4.950898711	
Cpo	\$89,309.72	
K1	4.8509	A.1
K2	-0.3973	
K3	0.1445	
Volume (m3/day)	0.293	
How many days?	2	
Total Volume (m3)	0.586	
Fm	1	A.3, CS
log10Fp	0.00	
Fp	1.00	
C1	0	
C2	0	A.2
C3	0	
Pressure (barg)	1.01	
B1	1.49	A.4
B2	1.52	
CBM	\$268,822.25	
CBM(2016)	\$366,261.85	

Number of Tanks	1
Total Cost	\$366,261.85

Table 42: Extruder Energy Balance

Nylon-6,6 Product (Hot)	
Mass Flowrate (lb/day)	259,271
Cp (Btu/lb F)	0.718
Tin (F)	495
T out (F)	100

Cooling Water Sprinkler (Cold)	
Mass Flowrate (lb/day)	1,750,755.19
Cp (Btu/lb F)	1
Tin (F)	60
T out (F)	102

Density of Water (lb/ft ³)	61.54
Volumetric Flowrate (gal/day)	212813.7665
Cooling Water (\$/1000 gallons)	5
Service Factor	0.9
Cost/day	\$1,064.07
Cost/year	\$349,546.61

Table 43: Extruder Utility Calculation

Extruder Utility Calculation	
lb Product/day	259270.54
Cost/lb (\$)	\$0.018
Cost/day (\$)	\$4,666.87
Cost/year (\$)	\$1,533,066.70
-includes ServF	

Table 44: Waste Treatment Utility Calculation

Waste Treatment Calculation	
Water Treatment Cost	\$5/1000 gallons
Water Treatment Cost (\$/gal)	\$0.0050
Water Treatment Cost (\$/lb)	\$0.0005981
Lb/day Steam	42038
Cost of Treatment (\$/day)	\$25.1423445
Cost (\$/year)	\$8,259
-includes ServF (Separate from Ut.)	

Table 45: Raw Material Costs

Material	Mass Flowrate (lb/year)	Cost/lb of Material	Cost/year (\$\$\$/year)
Adipic Acid	54,890,775.00	\$0.61	\$33,593,154
HMDA	43,648,588.00	\$1.12	\$48,886,419
Water	466,101.36	\$0.00106	\$494
Nitrogen	485,194.50	\$0.0033	\$1,601
Total Cost			\$82,481,668

Table 46: Manufacturing Costs for 100% and 67% Capacity Operation

100% Capacity

Fixed Capital Investment (FCI)	\$10,709,662.46
Direct Manufacturing Costs	
Raw Materials	\$82,481,668.07
Water Treatment	\$8,259.26
Utilities	\$3,228,737.41
Operating Labor	\$409,563.82
Direct Supervisory and Clerical Labor	\$73,721.49
Maintenance and Repairs	\$642,579.75
Operating Supplies	\$96,386.96
Laboratory Charges	\$61,434.57
Total Direct Manufacturing Costs	\$87,002,351.33
Fixed Manufacturing Costs	
Local Taxes and Insurance	\$342,709.20
Plant Overhead Costs	\$675,519.04
Total Fixed Manufacturing Costs	\$1,018,228.23
Total Costs	\$88,020,579.57

67% Capacity

Fixed Capital Investment (FCI)	\$10,709,662.46
Direct Manufacturing Costs	
Raw Materials	\$55,262,717.61
Water Treatment	\$5,533.70
Utilities	\$2,163,254.06
Operating Labor	\$409,563.82
Direct Supervisory and Clerical Labor	\$73,721.49
Maintenance and Repairs	\$642,579.75
Operating Supplies	\$96,386.96
Laboratory Charges	\$61,434.57
Total Direct Manufacturing Costs	\$58,715,191.97
Fixed Manufacturing Costs	
Local Taxes and Insurance	\$342,709.20
Plant Overhead Costs	\$675,519.04
Total Fixed Manufacturing Costs	\$1,018,228.23
Total Costs	\$59,733,420.20

```

d(X) / d(t) = ra*V/Nao #conversion equation for batch processes
X(0) = 0 #initial conversion
t(0) = 0 #initial time
t(f) = 6 #stop time
Cao = 24.5 #initial concentration of Adipid Acid (mol/L)
Nao = 285.85 #initial moles of Adipid Acid (mole)
k = 1.7353 #rate constant with units of (1/hr)
V = 36.25 #volume of reactor with units of (L)
Cb = Ca #equation relating concentrations of reactants
Ca = Cao*(1-X) #effect of conversion on concentration
ra = k*Ca*Cb #rate law for second order reaction, first order with respect to each reactant

# a = Adipic Acid
# b = HMDA

```

Figure 19: PolyMath Code

POLYMATH Report
 Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	24.5	0.0308738	24.5	0.0308738
2	Cao	24.5	24.5	24.5	24.5
3	Cb	24.5	0.0308738	24.5	0.0308738
4	k	1.7353	1.7353	1.7353	1.7353
5	Nao	285.85	285.85	285.85	285.85
6	ra	1041.614	0.0016541	1041.614	0.0016541
7	t	0	0	6.	6.
8	V	36.25	36.25	36.25	36.25
9	X	0	0	0.9987398	0.9987398

Differential equations

1 $d(X)/d(t) = ra \cdot V / Nao$
 conversion equation for batch processes

Explicit equations

- 1 $Cao = 24.5$
 initial concentration of Adipid Acid (mol/L)
- 2 $Nao = 285.85$
 initial moles of Adipid Acid (mole)
- 3 $k = 1.7353$
 rate constant with units of (1/hr)
- 4 $V = 36.25$
 volume of reactor with units of (L)
- 5 $Ca = Cao \cdot (1 - X)$
 effect of conversion on concentration
- 6 $Cb = Ca$
 equation relating concentrations of reactants
- 7 $ra = k \cdot Ca \cdot Cb$
 rate law for second order reaction, first order with respect to each reactant

General

Total number of equations	8
Number of differential equations	1
Number of explicit equations	7
Elapsed time	0.000 sec
Solution method	RKF_45
Step size guess. h	0.000001
Truncation error tolerance. eps	0.000001

Figure 20: PolyMath Report

Production of Nylon-6,6																
i*	0.15															
	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032
Year	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Production (Nylon-6,6) (lb)			42500000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000
Sales Price (Nylon-6,6) (\$/lb)			\$2.00	\$2.00	\$2.00	\$2.00	\$2.00	\$2.00	\$2.00	\$2.00	\$2.00	\$2.00	\$2.00	\$2.00	\$2.00	\$2.00
Sales Revenue	0	0	85,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000
Net Revenue	0	0	85,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000	170,000,000
Manufacturing Costs (\$)			(25,036,354)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)	(50,072,708)
Depreciation (60%)			(449,806)	(809,650)	(647,720)	(518,176)	(414,721)	(331,507)	(294,623)	(294,623)	(295,073)	(294,623)	(147,536)			
Depreciation (40%)				(299,871)	(539,767)	(431,814)	(345,451)	(276,481)	(221,005)	(196,415)	(196,415)	(196,715)	(196,415)	(98,358)		
Loss Forward																
Writeoff (60%)																
Writeoff (40%)																
Taxable income	0	0	59,513,840	118,817,771	118,739,804	118,977,302	119,167,120	119,319,304	119,411,664	119,436,254	119,435,804	119,435,954	119,583,340	119,828,934	119,927,292	119,927,292
Tax @ 40%	0	0	(23,805,536)	(47,527,108)	(47,495,922)	(47,590,921)	(47,666,848)	(47,727,722)	(47,764,666)	(47,774,501)	(47,774,322)	(47,774,382)	(47,833,336)	(47,931,574)	(47,970,917)	(47,970,917)
Net Income	0	0	35,708,304	71,290,662	71,243,883	71,386,381	71,500,272	71,591,582	71,646,999	71,661,752	71,661,482	71,661,572	71,750,004	71,897,360	71,956,375	71,956,375
Depreciation (60%)			449,806	809,650	647,720	518,176	414,721	331,507	294,623	294,623	295,073	294,623	147,536	0	0	0
Depreciation (40%)				299,871	539,767	431,814	345,451	276,481	221,005	196,415	196,415	196,715	196,415	98,358	0	0
Loss Forward																
Writeoff											0			0		
Working Capital																
Fixed Capital		(4,498,058)	(2,998,705)													
Cash Flow	0	(4,498,058)	33,159,404	72,400,183	72,431,370	72,336,371	72,260,444	72,199,570	72,162,626	72,152,790	72,152,970	72,152,910	72,093,956	71,995,718	71,956,375	71,956,375
Discount Factor	1.0000	0.9286	0.7993	0.6879	0.5921	0.5096	0.4387	0.3776	0.3250	0.2797	0.2407	0.2072	0.1783	0.1535	0.1321	0.1137
Discounted Cash Flow	0	(4,176,942)	26,503,317	49,806,258	42,887,338	36,864,785	31,697,044	27,258,948	23,449,967	20,180,414	17,369,385	14,950,083	12,857,236	11,051,343	9,506,876	8,182,159
NPV @i*	328,388,211															
DCFROR	701.2489															

FCI
\$7,496,763.72

60% of FCI incurred in 2018
40% occurred in 2019
Startup in July 2019
Half Year of Production in 2019

Figure 21: Cash Flow Sheet: Best Case Scenario

Production of Nylon-6,6																
i*	0.15															
	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032
Year	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Production (Nylon-6,6) (lb)			42500000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000	85000000
Sales Price (Nylon-6,6) (\$/lb)			\$1.04	\$1.04	\$1.04	\$1.04	\$1.04	\$1.04	\$1.04	\$1.04	\$1.04	\$1.04	\$1.04	\$1.04	\$1.04	\$1.04
Sales Revenue	0	0	44,200,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000
Net Revenue	0	0	44,200,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000	88,400,000
Manufacturing Costs (\$)			(62,655,993)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)	(125,311,986)
Depreciation (60%)			(835,354)	(1,503,637)	(1,202,909)	(962,327)	(770,196)	(615,656)	(547,157)	(547,157)	(547,992)	(547,157)	(273,996)			
Depreciation (40%)				(556,902)	(1,002,424)	(801,940)	(641,552)	(513,464)	(410,437)	(364,771)	(364,771)	(365,328)	(364,771)	(182,664)		
Loss Forward																
Writeoff (60%)																
Writeoff (40%)																
Taxable income	0	0	(19,291,346)	(38,972,525)	(39,117,319)	(38,676,252)	(38,323,733)	(38,041,105)	(37,869,579)	(37,823,913)	(37,824,749)	(37,824,470)	(37,550,753)	(37,094,650)	(36,911,986)	(36,911,986)
Tax @ 40%	0	0	7,716,539	15,589,010	15,646,928	15,470,501	15,329,493	15,216,442	15,147,832	15,129,565	15,129,899	15,129,788	15,020,301	14,837,860	14,764,794	14,764,794
Net Income	0	0	(11,574,808)	(23,383,515)	(23,470,392)	(23,205,751)	(22,994,240)	(22,824,663)	(22,721,748)	(22,694,348)	(22,694,849)	(22,694,682)	(22,530,452)	(22,256,790)	(22,147,191)	(22,147,191)
Depreciation (60%)			835,354	1,503,637	1,202,909	962,327	770,196	615,656	547,157	547,157	547,992	547,157	273,996	0	0	0
Depreciation (40%)				556,902	1,002,424	801,940	641,552	513,464	410,437	364,771	364,771	365,328	364,771	182,664	0	0
Loss Forward																
Writeoff										0			0			
Working Capital																
Fixed Capital		(8,353,537)	(5,569,024)													
Cash Flow	0	(8,353,537)	(16,308,479)	(21,322,976)	(21,265,058)	(21,441,485)	(21,582,492)	(21,695,543)	(21,764,154)	(21,782,420)	(21,782,086)	(21,782,197)	(21,891,684)	(22,074,126)	(22,147,191)	(22,147,191)
Discount Factor	1.0000	0.9286	0.7993	0.6879	0.5921	0.5096	0.4387	0.3776	0.3250	0.2797	0.2407	0.2072	0.1783	0.1535	0.1321	0.1137
Discounted Cash Flow	0	(7,757,178)	(13,034,878)	(14,668,715)	(12,591,253)	(10,927,224)	(9,467,160)	(8,191,152)	(7,072,479)	(6,092,325)	(5,243,602)	(4,513,271)	(3,904,163)	(3,388,378)	(2,926,087)	(2,518,357)
NPV @i*	(112,296,223)															
DCFROR	#NUM!															

FCI
\$13,922,561

60% of FCI incurred in 2018
40% occurred in 2019
Startup in July 2019
Half Year of Production in 2019

Figure 22: Cash Flow Sheet: Worst Case Scenario

Figure 23: Safety Data Sheet: Adipic Acid



Safety Data Sheet
(Adipic acid)

DATE PREPARED: 5/31/2012
REVISION NUMBER: 5/31/2012

Section 1 – Company Information

Parchem - fine & specialty chemicals
415 Huguenot Street
New Rochelle, NY 10801
 ☎ (914) 654-6800 📠 (914) 654-6899
 🌐 parchem.com ✉ info@parchem.com

EMERGENCY RESPONSE NUMBER:
 CHEMTEL - Parchem CCN# M1S0007152
 Toll Free US & Canada: (800)255-3924
 All other Origins: (813) 248-0585
 Collect Calls Accepted

Section 2 – Product Identification/ Information on Ingredients

PRODUCT NAME Adipic Acid
 CAS NUMBER 124-04-9
 SYNONYM Hexanedioic acid; 1,4-Butane Dicarboxylic Acid
 FORMULA HOOC(CH₂)₄COOH

PRODUCT	CAS NUMBER	% BY WEIGHT
Adipic acid	124-04-9	100%

Section 3 – Hazards Identification

Classification of the substance/preparation
 EC Classification Xi - Irritant
 Safety Phrase S22, S25, S26

Emergency Overview
 Appearance and Odor: White crystalline powder; characteristic odor

Warning Statements
 WARNING!
 MAY CAUSE EYE AND RESPIRATORY TRACT IRRITATION
 COMBUSTIBLE DUST - EXPLOSION POTENTIAL

Potential Health Effects
 Likely Routes of Exposure: Eye and skin contact, inhalation.
 EYE CONTACT: Moderately irritating to eyes. Dust may cause eye irritation as would any foreign material.
 SKIN CONTACT: No more than slightly irritating to skin. No more than slightly toxic if absorbed.
 INHALATION: Moderately irritating if inhaled.
 INGESTION: No more than slightly toxic if swallowed. Significant adverse health effects are not expected to develop if only small amounts (less than a mouthful) are swallowed.
 Refer to Section 11 for toxicological information.



Safety Data Sheet (Adipic acid)

DATE PREPARED: 5/31/2012
REVISION NUMBER: 5/31/2012

Section 4 – First Aid Measures

IF IN EYES, immediately flush with plenty of water. If easy to do, remove contact lenses. Get medical attention if irritation persists. Remove material from eyes, skin, and clothing. Wash heavily contaminated clothing before reuse.

IF ON SKIN, immediate first aid is not likely to be required. This material can be removed with soap and water.

IF INHALED, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Remove material from eyes, skin and clothing.

IF SWALLOWED, immediate first aid is not likely to be required. A physician or Poison Control Center can be contact for advice. Wash heavily contaminated clothing before reuse.

Section 5 – Fire Fighting Measures

Flash Point: 385° F (196° C) Method: Cleveland Open Cup

Fire Point: 450° F (232° C) Method: Cleveland Open Cup

Autoignition Temperature: 550° C

Hazardous Products of Combustion: As with any organic material, carbon dioxide, carbon monoxide, smoke and soot can be produced.

Extinguishing Media: In case of fire, use water spray (fog), foam, dry chemical, or CO₂.

Unusual Fire and Explosion Hazards: This material may contain enough fines to form an explosive mixture if mixed with a sufficient quantity of air.

Fire Fighting Equipment: Fire fighters and others exposed to products of combustion should wear self-contained breathing apparatus. Equipment should be thoroughly decontaminated after use.

Section 6 – Accidental Release Measures

Personal Precautions: Use personal protection recommended in Section 8.

Environmental Precautions: Keep out of drains and water courses.

Methods for Cleanup: In case of spill, do not blow material. Use vacuum equipment designed specifically for handling combustible dusts. Flush spill area with water.

Refer to Section 13 for disposal information and Sections 14 and 15 for reportable quantity information.

Section 7 – Handling & Storage

Avoid contact with eyes, skin and clothing.

Avoid breathing dust.

Keep container closed.

Use with adequate ventilation.

Wash thoroughly after handling.



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Keep away from heat, sparks and flame.
Avoid creating a dust cloud in handling, transfer and clean up.
Emptied container retains product residue. Observe all recommended safety precautions until container is cleaned, reconditioned, or destroyed. Do not cut or weld on or near this container, even when empty. Container retains vapor and product residue. The reuse of this material's container for non-industrial purposes is prohibited and any reuse must be in consideration of the data provided in the MSDS.

Section 8 – Exposure Controls & Personal Protection

EYE PROTECTION: Wear chemical goggles. Have eye flushing equipment available.
SKIN PROTECTION: Although this material does not present a significant skin concern, minimize skin contamination by following good industrial practice. Wearing of protective gloves is recommended. Consult the glove/clothing manufacturer to determine the appropriate type of glove/clothing for a given application. Wash contaminated skin thoroughly after handling.
RESPIRATORY PROTECTION: Avoid breathing dust. Use NIOSH/MSHA approved respiratory protection equipment when airborne exposure limits are exceeded (see below). Consult respirator manufacturer to determine appropriate type equipment for given application. Observe respirator use limitations specified by NIOSH/MSHA or the manufacturer. If used, full face-piece replaces the need for face shield and/or chemical goggles. Respiratory protection programs must comply with 29 CFR 1910.134.
VENTILATION: Provide natural or mechanical ventilation to control exposure levels below airborne exposure limits (see below). The use of local mechanical exhaust ventilation at sources of air contamination such as open process equipment is preferred. Consult NFPA Standard 91 for design of exhaust systems.

Airborne Exposure Limits:

<u>Product/Component</u>	<u>OSHA PEL</u>	<u>ACGIH TLV</u>
Adipic Acid	None Established	5 mg/m ³

Section 9 – Physical & Chemical Properties

Appearance: White crystalline powder
Autoignition Temperature: 550° C
Melting Point: 152° C
Boiling Point: 337.5° C
Solubility in Water: 19.0 g/L @ 20° C
830 g/L @ 90° C

NOTE: These physical data are typical values based on material tested but may vary from sample to sample. Typical values should not be construed as guaranteed analysis of any specific lot or as



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specifications for the product.

Section 10 – Stability & Reactivity Data

Stability: Product is stable under normal conditions of storage and handling.
Materials to Avoid: None known.
Conditions to Avoid: All sources of ignition.
Hazardous Polymerization: Does not occur.
Hazardous Decomposition Products: None known.

Section 11 – Toxicological Information

Data from Manufacturer's studies and from available scientific literature indicate the following:

Single dose (acute) studies indicate:

- Oral - Practically Nontoxic (Rat LD₅₀ - 5,050 mg/kg)
- Dermal - Practically Nontoxic (Rabbit LD₅₀ - >7,940 mg/kg)
- Eye Irritation - Moderately Irritating (Rabbit, 18.2/110.0)
- Skin Irritation - Practically Nonirritating (Rabbit, 4 hr. exposure, 0.0/8.0)

Repeat dose toxicity: rat, inhalation: No adverse effects reported in repeat dose studies.

Developmental Toxicity:

Mouse, diet: No birth defects were noted in rats given the active ingredient orally during pregnancy

Rat, diet: No birth defects were noted in rats given the active ingredient orally during pregnancy

Hamster, diet: No birth defects were noted in rats given the active ingredient orally during pregnancy

Carcinogenicity: Rat, diet, 24 months: No tumors.

Mutagenicity: No genetic effects were observed in standard tests using bacterial cells and whole animals.

This material has been defined as a hazardous chemical under the criteria of the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Section 12 – Ecological Information

Environmental Toxicity

Fish: 48h, LC₅₀ Rainbow trout (*oncorhynchus mykiss*) > 100 mg/L

96 h, LC₅₀ Fathead minnow (*pimephales promelas*) 97 mg/L



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Environmental Fate

Biodegradation: Readily biodegradable.

Section 13 – Disposal Consideration

This material when discarded is not a hazardous waste as that term is defined by the Resource, Conservation and Recovery Act (RCRA), 40 CFR 261. Dispose of by landfill, incineration or recycle in accordance with local, state and federal regulations. Consult your attorney or appropriate regulatory officials for information on such disposal.

This product should not be dumped, spilled, rinsed or washed into sewers or public waterways.

Section 14 – Transportation Data

The data provided in this section is for information only. Please apply the appropriate regulations to properly classify your shipment for transportation.

US DOT

Proper Shipping Name: Environmentally hazardous substances, solid, n.o.s. (adipic acid)*

Hazard Class: 9

Hazard Identification Number: UN3077

Packing Group: III

Transport Label: Class 9

Canadian TDG - Not Regulated

US DOT RQ: 5000 lbs adipic acid. Package size containing reportable amount: 5000 lbs.
Release of more than the Reportable Quantity to the environment in a 24 hour period requires notification to the National Response Center (800-424-8802 or 202-426-2675)

* Applies ONLY to containers which contain an RQ or RL.

Section 15 – Regulatory Information

EC Label

Hazard Symbol:	Xi - Irritant
R36	Irritating to eyes.
S22	Do not breathe dust.
S25	Avoid contact with eyes.
S26	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice



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Chemical Inventory

TSCA Inventory: Listed
 DSL Inventory: Listed
 EU: Listed
 Australia: Listed
 Korea: Listed
 Japan: Listed
 Philippines: Listed
 China: Listed

WHMIS Classification: D2(B) - Materials Causing Other Toxic Effects

SARA Hazard Notification

Hazard Categories Under Title III Rules (40 CFR 370):	Immediate
Section 302 Extremely Hazardous Substances:	Not Applicable
Section 313 Toxic Chemical(s):	Not Applicable

CERCLA Reportable Quantity: 5000 lbs

Refer to Section 11 for OSHA Hazardous Chemical(s) and Section 13 for RCRA classification

This product has been classified in accordance with the hazard criteria of the Canadian Controlled Products Regulation and the MSDS contains all the information required by the Canadian Controlled Products Regulation.

Section 16 – Other Information

	<u>Health</u>	<u>Fire</u>	<u>Reactivity</u>	<u>Additional Information</u>
Suggested NFPA Rating:	2	1	0	
Suggested HMIS Rating:	2	1	0	E

Disclaimer

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product.

Figure 24: Safety Data Sheet: HMDA

Safety Data Sheet
according to 29CFR1910/1200 and GHS Rev. 3

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Hexamethylenediamine,

SECTION 1 : Identification of the substance/mixture and of the supplier


Product name : Hexamethylenediamine,
Manufacturer/Supplier Trade name:
Manufacturer/Supplier Article number: S25350
Recommended uses of the product and uses restrictions on use:
Manufacturer Details:
AquaPhoenix Scientific
9 Barnhart Drive, Hanover, PA 17331


Supplier Details:
Fisher Science Education
15 Jet View Drive, Rochester, NY 14624

Emergency telephone number:
Fisher Science Education Emergency Telephone No.: 800-535-5053

SECTION 2 : Hazards identification

Classification of the substance or mixture:

 **Irritant**
Acute toxicity (oral, dermal, inhalation), category 4
Specific target organ toxicity following single exposure, category 3

 **Corrosive**
Skin corrosion, category 1B

Acute Tox. 4
Skin Corr. 1B
STOT SE 3
Hazards Not Otherwise Classified - Combustible Dust

Signal word :Danger

Hazard statements:
Harmful if swallowed
Harmful in contact with skin
Causes severe skin burns and eye damage
May cause respiratory irritation

Precautionary statements:
If medical advice is needed, have product container or label at hand
Keep out of reach of children
Read label before use
Do not breathe dust/fume/gas/mist/vapours/spray
Wash skin thoroughly after handling
Do not eat, drink or smoke when using this product
Use only outdoors or in a well-ventilated area
Wear protective gloves/protective clothing/eye protection/face protection
Immediately call a POISON CENTER or doctor/physician

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Hexamethylenediamine,

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting
 IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower
 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do.
 Continue rinsing
 Call a POISON CENTER or doctor/physician if you feel unwell
 Specific treatment (see supplemental first aid instructions on this label)
 Rinse mouth
 Wash contaminated clothing before reuse
 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
 Store locked up
 Store in a well ventilated place. Keep container tightly closed
 Dispose of contents and container to an approved waste disposal plant

Combustible Dust Hazard :
 May form combustible dust concentrations in air (during processing).

Other Non-GHS Classification:



Health	3
Flammability	2
Physical Hazard	1
Personal Protection	X

HMIS RATINGS (0-4)

SECTION 3 : Composition/information on ingredients

Ingredients:		
CAS 124-09-4	Hexamethylaminediamine	100 %
Percentages are by weight		

SECTION 4 : First aid measures

Description of first aid measures

- After inhalation:** Move exposed individual to fresh air. Loosen clothing as necessary and position individual in a comfortable position. Seek medical advice if discomfort or irritation persists. If breathing difficult, give oxygen.
- After skin contact:** Wash affected area with soap and water. Rinse/flush exposed skin gently using water for 15-20 minutes. Seek medical advice if discomfort or irritation persists.
- After eye contact:** Protect unexposed eye. Rinse/flush exposed eye(s) gently using water for 15-20 minutes.

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Hexamethylenediamine,

Remove contact lens(es) if able to do so during rinsing. Seek medical attention if irritation persists or if concerned.

After swallowing: Rinse mouth thoroughly. Do not induce vomiting. Have exposed individual drink sips of water. Seek immediate medical attention or advice.

Most important symptoms and effects, both acute and delayed:

Irritation, Nausea, Headache, Shortness of breath.;

Indication of any immediate medical attention and special treatment needed:

If seeking medical attention, provide SDS document to physician.

SECTION 5 : Firefighting measures

Extinguishing media

Suitable extinguishing agents: If in laboratory setting, follow laboratory fire suppression procedures. Use appropriate fire suppression agents for adjacent combustible materials or sources of ignition

For safety reasons unsuitable extinguishing agents:

Special hazards arising from the substance or mixture:

Combustion products may include carbon oxides or other toxic vapors. Thermal decomposition can lead to release of irritating gases and vapors. Avoid generating dust; fine dust dispersed in air in sufficient concentrations, and in the presence of an ignition source is a potential dust explosion hazard.

Advice for firefighters:

Protective equipment: Use NIOSH-approved respiratory protection/breathing apparatus.

Additional information (precautions): Move product containers away from fire or keep cool with water spray as a protective measure, where feasible. Use spark-proof tools and explosion-proof equipment.

SECTION 6 : Accidental release measures

Personal precautions, protective equipment and emergency procedures:

Wear protective equipment. Transfer to a disposal or recovery container. Use spark-proof tools and explosion-proof equipment. Use respiratory protective device against the effects of fumes/dust/aerosol. Keep unprotected persons away. Ensure adequate ventilation. Keep away from ignition sources. Protect from heat. Stop the spill, if possible. Contain spilled material by diking or using inert absorbent.

Environmental precautions:

Prevent from reaching drains, sewer or waterway. Collect contaminated soil for characterization per Section 13

Methods and material for containment and cleaning up:

If in a laboratory setting, follow Chemical Hygiene Plan procedures. Place into properly labeled containers for recovery or disposal. If necessary, use trained response staff/contractor. Dust deposits should not be allowed to accumulate on surfaces, as these may form an explosive mixture if they are released into the atmosphere in sufficient concentration. Avoid dispersal of dust in the air (i.e., clearing dust surfaces with compressed air). Collect solids in powder form using vacuum with (HEPA filter)

Reference to other sections:

SECTION 7 : Handling and storage

Precautions for safe handling:

Minimize dust generation and accumulation. Wash hands after handling. Routine housekeeping should be instituted to ensure that dusts do not accumulate on surfaces. Dry powders can build static electricity charges when subjected to the friction of transfer and mixing operations. Follow good hygiene procedures when handling chemical materials. Do not eat, drink, smoke, or use personal products when handling chemical substances. Use only in well ventilated areas. Avoid contact with eyes, skin, and clothing.

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Hexamethylenediamine,

Conditions for safe storage, including any incompatibilities:

Store in a cool location. Provide ventilation for containers. Avoid storage near extreme heat, ignition sources or open flame. Store away from foodstuffs. Store away from oxidizing agents. Keep container tightly sealed. Store with like hazards. Do not store in metal containers.

SECTION 8 : Exposure controls/personal protection



Control Parameters:

124-09-4, Hexamethylaminodiamine, ACGIH TLV TWA 0.5 ppm

Appropriate Engineering controls:

Emergency eye wash fountains and safety showers should be available in the immediate vicinity of use/handling. Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapor or dusts (total/respirable) below the applicable workplace exposure limits (Occupational Exposure Limits-OELs) indicated above. Use under a fume hood. It is recommended that all dust control equipment such as local exhaust ventilation and material transport systems involved in handling of this product contain explosion relief vents or an explosion suppression system or an oxygen deficient environment. Ensure that dust-handling systems (such as exhaust ducts, dust collectors, vessels, and processing equipment) are designed in a manner to prevent the escape of dust into the work area (i.e., there is no leakage from the equipment).

Respiratory protection:

Not required under normal conditions of use. Use suitable respiratory protective device when high concentrations are present. Use suitable respiratory protective device when aerosol or mist is formed. For spills, respiratory protection may be advisable.

Protection of skin:

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation being used/handled. Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation.

Eye protection:

Safety glasses with side shields or goggles.

General hygienic measures:

The usual precautionary measures are to be adhered to when handling chemicals. Keep away from food, beverages and feed sources. Immediately remove all soiled and contaminated clothing. Wash hands before breaks and at the end of work. Do not inhale gases/fumes/dust/mist/vapor/aerosols. Avoid contact with the eyes and skin.

SECTION 9 : Physical and chemical properties

Appearance (physical state,color):	White solid	Explosion limit lower:	Not Determined
		Explosion limit upper:	Not Determined
Odor:	Fish - like weak odor	Vapor pressure:	3mmHg @60C
Odor threshold:	Not Determined	Vapor density:	4.0 (air=1)
pH-value:	12.1% aq. sol	Relative density:	0.848 (water=1)
Melting/Freezing point:	38 - 41 C	Solubilities:	Material is water soluble.

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Hexamethylenediamine,

Boiling point/Boiling range:	204C	Partition coefficient (n-octanol/water):	Not Determined
Flash point (closed cup):	250 C	Auto/Self-ignition temperature:	Not Determined
Evaporation rate:	Not Determined	Decomposition temperature:	Not Determinedn
Flammability (solid,gaseous):	Not Determined	Viscosity:	a. Kinematic:Not Determined b. Dynamic: Not Determined
Density: Not Determined Hexamethylaminediamine: Molecular Weight: 116.20			

SECTION 10 : Stability and reactivity

Reactivity:

Chemical stability:No decomposition if used and stored according to specifications.

Possible hazardous reactions:None under normal processing.

Conditions to avoid:Store away from oxidizing agents, strong acids or bases.High temperatures, moisture, metals, ignition sources, strong oxidants.

Incompatible materials:Strong oxidizing agents.nitric acid

Hazardous decomposition products:Oxides of carbon, oxides of nitrogen.

SECTION 11 : Toxicological information

Acute Toxicity:	
Oral:	750 mg/kg LD50 orl - rat
Chronic Toxicity: No additional information.	
Corrosion Irritation: No additional information.	
Sensitization:	No additional information.
Single Target Organ (STOT):	No additional information.
Numerical Measures:	No additional information.
Carcinogenicity:	No additional information.
Mutagenicity:	No additional information.
Reproductive Toxicity:	May cause fetal effects based on animal studies .

SECTION 12 : Ecological information

Ecotoxicity Persistence and degradability: Readily degradable in the environment.

Bioaccumulative potential:

Mobility in soil:

Other adverse effects:

SECTION 13 : Disposal considerations

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Hexamethylenediamine,

Waste disposal recommendations:

Product/containers must not be disposed together with household garbage. Do not allow product to reach sewage system or open water. It is the responsibility of the waste generator to properly characterize all waste materials according to applicable regulatory entities (US 40CFR262.11). Consult federal state/ provincial and local regulations regarding the proper disposal of waste material that may incorporate some amount of this product.

SECTION 14 : Transport information

UN-Number

2280

UN proper shipping name

Hexamethylenediamine

Transport hazard class(es)



Class:

8 Corrosive substances

Packing group:III

Environmental hazard:

Transport in bulk:

Special precautions for user:

SECTION 15 : Regulatory information

United States (USA)

SARA Section 311/312 (Specific toxic chemical listings):

Acute, Chronic

SARA Section 313 (Specific toxic chemical listings):

None of the ingredients is listed

RCRA (hazardous waste code):

None of the ingredients is listed

TSCA (Toxic Substances Control Act):

All ingredients are listed.

CERCLA (Comprehensive Environmental Response, Compensation, and Liability Act):

None of the ingredients is listed

Proposition 65 (California):

Chemicals known to cause cancer:

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for females:

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for males:

None of the ingredients is listed

Chemicals known to cause developmental toxicity:

None of the ingredients is listed

Canada

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Hexamethylenediamine,

Canadian Domestic Substances List (DSL):

All ingredients are listed.

Canadian NPRI Ingredient Disclosure list (limit 0.1%):

None of the ingredients is listed

Canadian NPRI Ingredient Disclosure list (limit 1%):

124-09-4 Hexamethylaminodiamine

SECTION 16 : Other information

This product has been classified in accordance with hazard criteria of the Controlled Products Regulations and the SDS contains all the information required by the Controlled Products Regulations. Note: The responsibility to provide a safe workplace remains with the user. The user should consider the health hazards and safety information contained herein as a guide and should take those precautions required in an individual operation to instruct employees and develop work practice procedures for a safe work environment. The information contained herein is, to the best of our knowledge and belief, accurate. However, since the conditions of handling and use are beyond our control, we make no guarantee of results, and assume no liability for damages incurred by the use of this material. It is the responsibility of the user to comply with all applicable laws and regulations applicable to this material.

GHS Full Text Phrases:

Abbreviations and acronyms:

IMDG: International Maritime Code for Dangerous Goods

PNEC: Predicted No-Effect Concentration (REACH)

CFR: Code of Federal Regulations (USA)

SARA: Superfund Amendments and Reauthorization Act (USA)

RCRA: Resource Conservation and Recovery Act (USA)

TSCA: Toxic Substances Control Act (USA)

NPRI: National Pollutant Release Inventory (Canada)

DOT: US Department of Transportation

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

ACGIH: American Conference of Governmental Industrial Hygienists

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMIS: Hazardous Materials Identification System (USA)

WHMIS: Workplace Hazardous Materials Information System (Canada)

DNEL: Derived No-Effect Level (REACH)

Effective date : 01.23.2015

Last updated : 03.19.2015

Figure 25: Safety Data Sheet: Nylon-6,6



Ensinger
385 Meadowlands Blvd.
Washington, PA 15301
Ph: 724-746-6050
F: 724-746-9209

Ensinger
1 Main Street
Grenloch, NJ 08032
Ph: 856-227-0500
F: 856-232-1754

MATERIAL SAFETY DATA SHEET		
TECAMID™ Nylon 6/6 & TECAMID™ HS Nylon 6/6		
EMERGENCY TELEPHONE:	724-746-6050 or 856-227-0500	
Issue Date:	September 1, 1985	
Revised Date:	January 1, 2010	
TRADE NAME:	Nylon 6/6 Natural, Heat Stabilized	
CHEMICAL NAME:	Polyhexamethylene adipamide	
1. Composition/ Ingredient Information		
Material	CAS Number	Percent, %
Nylon 6/6	32131-17-2	>98%
Lubricants & Stabilizers		<2%
<i>Material is not known to contain Toxic Chemicals under Section 303 of Title III of the Superfund Amendments and Reauthorization Act of 1986 and 40 CFR part 372.</i>		
2. Hazards Identification		
<p>POLYHEXAMETHYLENE ADIPAMIDE In general, skin irritation hasn't been produced in human patch tests with nylon 6/6. However, a small percentage of subjects may respond to prolonged contact with skin redness. Significant skin permeation, and systemic toxicity, after contact appears unlikely. There are no reports of human sensitization.</p> <p>If particles of nylon 6/6 contact the eye, mechanical irritation with tearing, pain or blurred vision may result.</p> <p>Carcinogenicity information None of the components present in this material at concentrations equal to or greater than 0.1% are listed by IARC, NTP, OSHA, or ACGIH as a carcinogen.</p>		
3. First Aid Measures		
<p>Inhalation: No specific intervention is indicated as the compound is not likely to be hazardous by inhalation. Consult a physician if necessary. If exposed to fumes from overheating or combustion, move to fresh air. Consult a physician if symptoms persist.</p> <p>Skin Contact: The compound is not likely to be hazardous by skin contact but cleansing the skin after use is advisable. If molten polymer gets on skin, cool rapidly with cold water. Do not attempt to peel polymer from skin. Obtain medical treatment for thermal burn.</p> <p>Eye Contact: In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Call a physician if necessary.</p> <p>Ingestion: No specific intervention is indication as compound is not likely to be hazardous by ingestion.</p>		
4. Fire Fighting Measures		
<p>Flammable Properties Flash Point Not Applicable Large molten masses may ignite spontaneously in air. Water quenching of such masses is good practice.</p> <p>Fire & Explosion Hazards Like most organic materials in powder form, dust generated from this product may form a flammable dust-air mixture. Potential for a dust explosion may exist. Minimize the generation and accumulation of dust. Keep away from sources of ignition Hazardous gases/vapors produced in fire are ammonia, carbon monoxide, traces of hydrogen cyanide, and aldehydes.</p>		

<p>Extinguishing Media Water, Foam, Dry Chemical, CO2</p> <p>Fire Fighting Instructions Keep personnel removed and upwind of fire. Wear self-contained breathing apparatus.</p>													
5. Accidental Release Measures													
<p>Handling: Minimize the generation and accumulation of dust. Storage: Store in a cool, dry place. Keep containers tightly closed to prevent moisture absorption and contamination.</p>													
6. Exposure Controls / Personal Protection													
<p>Engineering Controls: VENTILATION When hot processing this material, use local and/or general exhaust ventilation to control the concentration of vapors and fumes below exposure limits In cutting or grinding operations with the material, use local exhaust to control the concentration of dust below exposure limits.</p> <p>Personal Protective Equipment Eye/Face protection: Wear safety glasses. Wear coverall chemical splash goggles and face shield when possibility exists for eye or face contact due to splashing or spraying of molten material. A full face mask positive pressure air supplied respirator provides protection from eye irritation. Respirators: A NIOSH/MSHA approved air purifying respirator with an organic vapor cartridge with a dust/mist filter may be permissible under certain circumstances where airborne concentrations are expected to exceed exposure limits. Use a positive pressure air supplied respirator if there is any potential for an uncontrolled release, exposure levels are not known, or any other circumstances where air purifying respirators may not provide adequate protection. During grinding, sawing routing, drilling or sanding operations use a NIOSH/MSHA approved air purifying respirator with dust/mist cartridge or canister if airborne particulate concentrations are expected to exceed permissible exposure levels. Protective Clothing: If there is potential contact with hot/molten material, wear heat resistant clothing and footwear. Wear leather or cotton gloves when grinding, sawing, routing, drilling or sanding.</p> <p>Exposure Guidelines Exposure Limits</p> <table border="0"> <tr> <td>Nylon 6/6</td> <td></td> </tr> <tr> <td>PEL (OSHA)</td> <td>None Established</td> </tr> <tr> <td>TLV (ACGIH)</td> <td>None Established</td> </tr> <tr> <td>AEL (DuPont)</td> <td>10 mg/m3, 8 Hr TWA, total dust</td> </tr> <tr> <td></td> <td>5 mg/m3, 8 Hr TWA, respirable dust</td> </tr> </table>		Nylon 6/6		PEL (OSHA)	None Established	TLV (ACGIH)	None Established	AEL (DuPont)	10 mg/m3, 8 Hr TWA, total dust		5 mg/m3, 8 Hr TWA, respirable dust		
Nylon 6/6													
PEL (OSHA)	None Established												
TLV (ACGIH)	None Established												
AEL (DuPont)	10 mg/m3, 8 Hr TWA, total dust												
	5 mg/m3, 8 Hr TWA, respirable dust												
7. Physical and Chemical Properties													
<p>Physical Data</p> <table border="0"> <tr> <td>Melting Point</td> <td>>200 C (392 F)</td> </tr> <tr> <td>Solubility in H2O</td> <td>Insoluble</td> </tr> <tr> <td>Odor</td> <td>None</td> </tr> <tr> <td>Form</td> <td>Stock Shapes</td> </tr> <tr> <td>Specific Gravity</td> <td>>1.0</td> </tr> <tr> <td>Color</td> <td>Natural (off-white) or Black</td> </tr> </table>		Melting Point	>200 C (392 F)	Solubility in H2O	Insoluble	Odor	None	Form	Stock Shapes	Specific Gravity	>1.0	Color	Natural (off-white) or Black
Melting Point	>200 C (392 F)												
Solubility in H2O	Insoluble												
Odor	None												
Form	Stock Shapes												
Specific Gravity	>1.0												
Color	Natural (off-white) or Black												
8. Stability & Reactivity													
<p>Chemical Stability: Stable at normal temperatures and storage conditions Conditions to Avoid: Temperatures above 340C (644 F) Incompatibility with Other Materials: Incompatible or can react with strong acids , oxidizing agents Decomposition: Hazardous gasses or vapors can be released including ammonia, carbon monoxide, cyclopentanone, hydrogen cyanide, nitrogen oxides. Polymerization: Polymerization will not occur</p>													
9. Toxicological Information													

Animal Data

Nylon 6/6: Oral LD50, rat: > 10,000 mg/kg

Nylon 6/6 is not a skin irritant in tests with animals.

Single exposure by ingestion to high doses cause decreased body weight. Long term exposure cause no significant toxicological effects.

repeated inhalation exposure caused histopathological changes of the lungs and kidneys.

In animal testing Nylon 6/6 has not caused carcinogenicity. No animal data are available to define developmental, reproductive, or mutagenic hazards.

10. Ecological Information

Ecotoxicological Information

Aquatic Toxicity: No information is available. Toxicity is expected to be low based on insolubility in water. Do not discharge to streams, ponds, lakes, or sewers

11. Disposal Consideration

Waste Disposal: Preferred options for disposal are (1) recycling, (2) incineration with energy recovery, and (3) landfill. The high fuel value of this product makes option 2 very desirable for material that cannot be recycled but incinerator must be capable of scrubbing out acidic combustion products. Treatment, storage, transportation, and disposal must be in accordance with applicable federal, state/provincial, and local regulations.

12. Transportation Information

Shipping Information: Not regulated by transportation by DOT/IMO/IATA.

13. Regulatory Information

U.S. Federal Regulations

TSCA Inventory Status In compliance with TSCA Inventory requirements for commercial purposes.

State Regulations (U.S.)

State Right to Know Laws

No substances on the state hazardous substances list, for the states indicated below, are used in the manufacture of products listed on the Material Safety Data Sheet.

Substances on the Pennsylvania Hazardous Substances List Present at a Concentration of 1% or more (0.01% for special hazardous substances): None known

Warning: Substances known to the state of California to cause cancer, birth defects, or other reproductive harm: None known

Substances on the New Jersey workplace hazardous substance list present at a concentration of 1% or more (0.1% for substances identified as carcinogens, mutagens, or teratogens): None Known

14. Other Information

Additional Information

Medical Use: CAUTION: Do not use in medical applications involving permanent implantation in the human body.

This material safety data sheet and the information it contains is offered to you in good faith as accurate. We have reviewed any information contained in this data sheet which we received from sources outside our company. We believe this information to be correct but cannot guarantee its accuracy or completeness. Health and safety precaution in this data sheet may not be adequate for all individuals and/or situations. It is the user's obligation to evaluate and use this product safely and to comply with all applicable laws and regulation. No statement made in the data sheet shall be construed as a permission or recommendation for the use of any product in a manner that might infringe existing patents. No warranty is made, either express or implied.

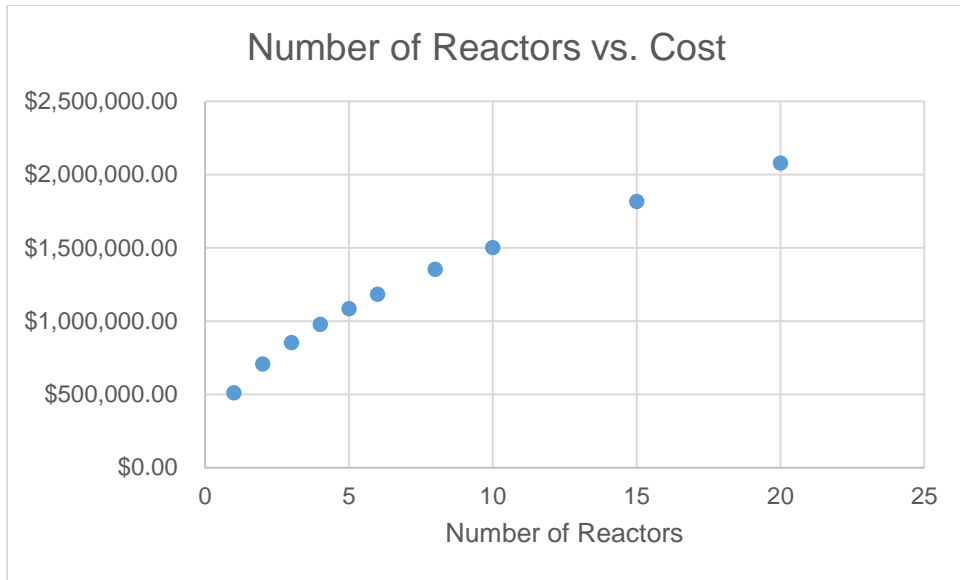


Figure 26: Number of Reactors vs. Cost