MEMORANDUM

Date: March 9, 2017
To: AIChE Competition Chairs
From: Group #_____
Subject: AIChE 2017 Student Design Competition Nylon 6 6 Grassroots Plant Design

As requested on February 7, 2017, a preliminary design for a Nylon 6 6 grassroots facility to produce nylon granules through an extrusion process has been completed.

The process of achieving 85 MM lb/yr of Nylon 6 6 granules is described in the following report. Through a continuous process, a net present value of $12,916,000, and a discounted cash flow rate of return of 30.4% were determined. This project is recommended due to the economic evaluation of a ten year project life. Additional sizing and costing of equipment as well as a preliminary safety and hazard analysis are included in this report.

If any of the following information needs further explanation, please contact this design group.

AIChE Design Project: Grassroots Nylon 6 6 Plant

Group #_____

March 9, 2017

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Abstract
A preliminary design of a Nylon 6 6 plant to produce granules by extrusion was conducted for Calvert City, Kentucky. This process involves a reaction between adipic acid and hexamethylene diamine (HMDA) through a continuous process. This type of process was chosen over a batch process to make the system inherently safer, reduce process time, and decrease operating costs [1]. Through the use of a continuous polymerization reactor, molten Nylon is produced and then processed by an extruder and additional mechanical processing equipment to dry the Nylon granules. The production of Nylon granules was chosen instead of Nylon filaments. This is due to the versatility of the Nylon granules to be further processed into different lengths and thicknesses based on the customers' specific needs.

The economic evaluation for the Nylon production process is summarized in *Table 1*.

Table 1: Nylon 6,6 Plant Economic Analysis	
Net Present Value	$12,916,000
Discounted Cash Flow Rate of Return	30.4%
Undiscounted Payback Period	4.11 years

The net present value of the project was calculated to be $12,916,000 with a discounted cash flow rate of return (DCFROR) of 30.4%. The DCFROR is greater than the hurdle rate of 15% which makes this project economically attractive. The payback period is 4.11 years for a ten year project life.

This process has some safety concerns based on the polymerization reactor and components involved in the process, but these risks will be controlled. Cooling jackets, alarms, and other emergency procedures will be implemented to ensure the safety of everyone involved with the plant and the surrounding community.

Introduction

Nylon 6 6 is a strong and versatile polymer that has many uses throughout different industries. This makes it useful to study innovative and sustainable ways to produce it in bulk. Because Nylon 6 6 has such versatile applications, it can be produced as granules to be processed by other manufacturers or made into fibers for textile applications. The intent of this design project was to design a manufacturing facility for Nylon 6 6 in order to determine the profitability of producing 85 MMlbs/yr of Nylon while considering safety, sustainability, demand and process control.

The following report shows the analysis of a grassroots industrial facility that produces Nylon 6 6 granules in a continuous process. The granules are produced from adipic acid and HMDA in a polycondensation reaction. This is done through the use of mixers, a crystallizer, and a continuous stirred tank reactor. The molten Nylon is extruded and cut into granules for sale.

To fully understand the scope of this process, a safety concept was evaluated for all equipment and potential hazards. Inherent safety is incorporated into the design, and a hazard analysis along with a preliminary hazard and operability study were completed for the process. This also provided the means to assess environmental concerns and loss prevention throughout the design. A control strategy was evaluated for the entire process to assist with the safety and ensure that the design was feasible. An economic analysis was performed for the production of Nylon 6 6 granules at the full capacity of 85 MMlbs/yr as well as a turndown case at 67% by considering the net present value and discounted cash flow rate of return (DCFROR). By using all of these separate concepts, it was possible to evaluate a cohesive design of the Nylon manufacturing facility.

The time line of this project started with research of previous Nylon producing processes to determine the specific equipment necessary, reaction mechanism and kinetics for the polymerization of Nylon 6 6. Next, the reaction kinetics were used to create simulations of the process using Polymath. Mass and energy balances could then be solved, leading to equipment sizing and costing. Revisions to the process were considered for safety and optimization. The economic analysis was then completed.

Process Flow Diagram and Material Balances

The following page provides a process flow diagram for the Nylon 6 6 formation process. The streams are labeled and the stream summary table is provided on the same page to provide ease when identifying the pressure, temperature, total mass flow rate, and component mass flow rates of each of the streams.

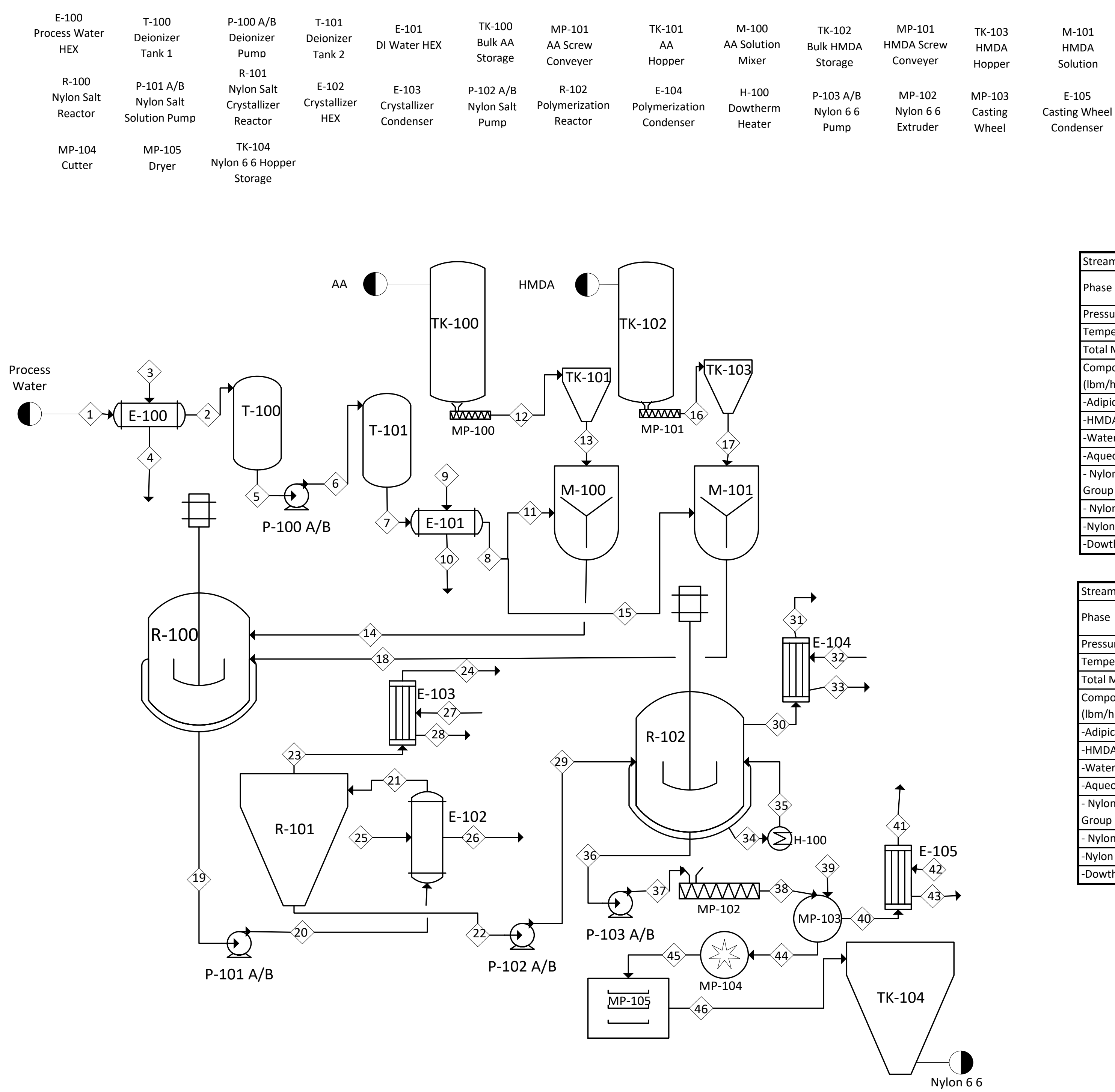

Figure 1: PFD of Nylon 6 6 Process

Table 2: Stream Summary Table of Nylon 6 6 Process

Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
Phase	Liquid	Liquid	Sat. Vapor	Sat. Liquid	Liquid	Liquid	Liquid	Liquid	Sat. Vapor	Sat. Liquid	Liquid	Solid	Solid	Liquid	Liquid	Solid	Solid	Liquid	Liquid/ Precipitate	Liquid/ Precipitate	Liquid/ Precipitate	Liquid/ Precipitate	Sat. Vapor
Pressure (psia)	108.9	103.9	189.7	189.7	95	103.9	95	90	189.7	189.7	90	14.7	14.7	90	90	14.7	14.7	90	90	196	191	189	182
Temperature (°F)	52	100.4	377	377	100.4	100.4	100.4	122	377	377	122	70	70	122	122	70	70	122	122	122	374	374	374
Total Mass Flow Rate (lbm/hr)	104,466	104,466	5,943	5,943	104,466	104,466	104,466	104,466	2,652	2,652	95,583	7,200	7,200	102,783	8,883	5,726	5,726	14,609	117,392	117,392	117,392	13,813	103,579
Component Mass Flow Rate (lbm/hr)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-Adipic Acid	0	0	0	0	0	0	0	0	0	0	0	7,200	7,200	7,200	-	0	0	0	0	0	0	0	0
-HMDA	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5,726	5,726	5,726	0	0	0	0	0
-Water	104,466	104,466	5,943	5,943	104,466	104,466	104,466	104,466	2,652	2,652	95,583	0	0	95,583	8,883	0	0	8,883	0	0	0	887	103,579
-Aqueous Nylon Salt Solution	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	117,392	117,392	117,392	0	0
- Nylon Salt - Carboxyl End Group	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7,200	0
- Nylon Salt - Amine End Group	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5726	0
-Nylon 6 6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-Dowtherm	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Stream Number	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46
Phase	Sat. Vapor	Sat. Liquid	Sat. Vapor	Sat. Liquid	Liquid	Liquid	Liquid/ Precipitate	Vapor	Sat. Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Sat. Vapor	Sat. Liquid	Liquid	Liquid	Solid	Solid	Solid
Pressure (psia)	182	182	614.7	614.7	100	100	252	250	250	100	100	152.7	152.7	250	1000	1000	100	14.7	14.7	100	95	14.7	14.7	9.7
Temperature (°F)	374	374	489	489	86	113	374	514.6	204.8	86	113	532.6	527	514.6	514.6	514.6	86	212	212	86	113	257	257	158
Total Mass Flow Rate (lbm/hr)	103,579	103,579	16,641	16,641	3.67E+06	3.67E+06	13,813	1,700	1,700	60,325	60,325	34,049	34,049	11,302	11,302	11,302	1,003	2,091	2,091	7.51E+04	7.51E+04	10,214	10,214	10,214
Component Mass Flow Rate (lbm/hr)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-Adipic Acid	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-HMDA	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
-Water	103,579	103,579	16,641	16,641	3.67E+06	3.67E+06	887	1,700	1,700	60,325	60,325	0	0	0	0	0	1,003	1,003	1,003	7.51E+04	7.51E+04	0	0	0
-Aqueous Nylon Salt Solution	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	606	606	0	0	0	0	0
- Nylon Salt - Carboxyl End Group	0	0	0	0	0	0	7,200	0	0	0	0	0	0	606	606	606	0	482	482	0	0	0	0	0
- Nylon Salt - Amine End Group	0	0	0	0	0	0	5726	0	0	0	0	0	0	482	482	482	0	0	0	0	0	0	0	0
-Nylon 6 6	0	0	0	0	0	0	0	0	0	0	0	0	0	10,214	10,214	10,214	0	0	0	0	0	10,214	10,214	10,214
-Dowtherm	0	0	0	0	0	0	0	0	0	0	0	34,049	34,049	0	0	0	0	0	0	0	0	0	0	0

The pressure was determined for each of the streams in Table 2 based on the assumption that there were no line losses in the system. This was due to the lack of information of the spatial layout of the plant during this preliminary design. A pressure drop of 5 psi was assumed across each condenser and heat exchanger [2]. However, the hydrostatic pressure was estimated based on the known height of the pieces of equipment. In addition, it is assumed the total mass flow rate of the material coming into each of the pieces of equipment is equal to the mass flow exiting the equipment, except for the material entering and exiting the polymerization reactor, R-102, which are streams 29, 30, and 36. In this piece of equipment, there is a generation term for the Nylon 6 6 reaction. Thus, the material balance is characterized by Equations 1 and is developed more specifically for this continuous process in Equation 2:

$$Input - Output + Generation = Accumulation \tag{1}$$

$$F_{In} - F_{Out} + rV = 0 \tag{2}$$

Where:

F_{In} is equal to the molar flow rate of the component in
F_{Out} is equal to the molar flow rate of the component coming out
r is the reaction rate
V is the volume of the fluid within the reactor

The V term is constant due to the assumption that the reactor is well-mixed and therefore has no spatial variation. This was done for each of the components of the polycondensation reaction (amine end group in Nylon salt solution, carboxyl end group in Nylon salt solution, Nylon 6 6, and water). There is no accumulation term because the process is assumed to be at steady state.

Process Description

The process discussed in this report converts the solid raw materials of adipic acid and HMDA to solid Nylon 6 6 granules. A simple block flow diagram is provided below to illustrate the main subsystems within this process.

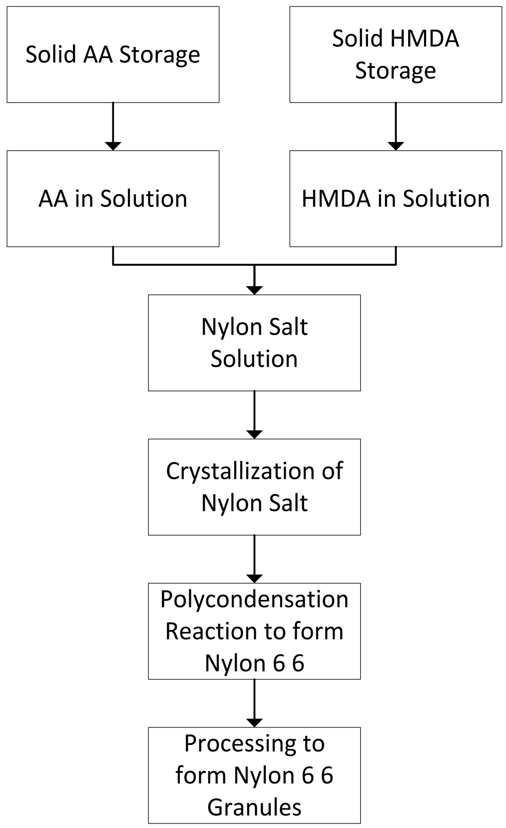

Figure 2: Block Flow Diagram of Nylon 6 6 Process

To begin, the solid raw materials must both be stored onsite in bulk in order to keep the process running continuously. Next, these solids are formed into adipic acid and HMDA solutions by mixing them with deionized water. The solids are dispensed into the mixers by hoppers. The deioinized water is crucial to eliminate the potential interaction of other ions with the adipic acid and HMDA ions later on in the formation of the Nylon salt. The amount of DI water is calculated to ensure that the solids are completely dissolved so that it can be assumed that the solutions are equimolar. These solutions are then added in equimolar amounts into the Nylon salt formation reactor. The Nylon salt solution formation is assumed to be instantaneous, thus the solution is simply mixed before moving to the crystallizer. In the crystallizer, the excess water within the Nylon salt solution is evaporated so that it is ready for the polycondensation reaction process. The polycondensation reactor is used to heat the solution to a temperature that causes the carboxyl and amine end groups of the adipic acid and HMDA to form polymer chains. As this process is happening, the byproduct of water is created and evaporated. Finally, the molten Nylon created from this reactor is processed through several pieces of equipment, including an extruder, casting wheel, chopper, and dryer, to create the final product of the Nylon granules for storage [3].

Energy Balance and Utility Requirements

The first utility used in the production of Nylon 6 6 is the process water that is converted to DI water. The cost of this utility per year was calculated based on the total mass flow rate of water needed to dissolve the solid adipic acid and HMDA in the system. This flow rate and price was minimized by increasing the temperature of the water from 52°F to 122°F to make the raw materials more soluble in the water. Therefore, less water will be required to dissolve the same mass of solids at this temperature than for room temperature water. In addition to this, cooling water will be introduced to the molten Nylon 6 6 on the casting wheel to cool it from about 515°F to 257°F. The final use for cooling water within the system will be to condense the water vapor produced in both the crystallization process and the polymerization reaction as well as the water vapor flashed off of the casting wheel.

Steam will also be utilized in this system to heat the process streams when needed. The points at which this is required is before the deionizer system, E-100, as well as for the crystallizer, E-102. The crystallization process requires a larger heat duty than does the process water used in mixing with the raw materials, thus high pressure steam is used on the side of the crystallizer, E-102. However, to minimize costs, medium pressure steam was used for the process water heat exchangers, E-100 and E-101. On the other hand, steam was not selected to be used to heat the polymerization reactor, R-102. This is because high pressure steam is not able to provide the desired heat duty to produce the molten Nylon. Thus, Dowtherm was selected to be used to provide continuous heating to this reaction [2]. It was decided that this will be a safer and more economical choice because Dowtherm causes less fouling in the heat exchanger and is not required to be at as high of a pressure as saturated steam.

In addition, electricity will be used to provide power to several pieces of equipment. These include the pumps and the drives required to operate the mixers, agitated reactors, screw conveyers, extruder, casting wheel, chopper, and dryer [2].

The utility requirements for this process are such that a large quantity of water must be treated. This is because water will be used and evaporated out of the process stream. Thus, since this water will come into contact with adipic acid and HMDA, the water should not be reused in the process because it has the potential to make the equimolar ratio of these two ions skewed. Additionally, exposure should be limited to the environment [4,5]. Also, it was assumed that this Nylon 6 6 producing plant would recycle cooling water and condensed steam to where solids would build up within the lines and need to be blown down. Thus, it was estimated that this blow down percentage would be 6% [6]. This water containing solids that is removed from the system will be treated to remove the solids before being disposed. Tertiary treatment was selected [2].

It is important to note that all of the values for both mass flow and cost per year of the utilities are calculated based on a service factor of 0.95. Also, the process water cost was determined using a public service commission from the Kentucky government [7]. The cost for remaining utilities were found using [2]. These prices are summarized in Table 3 below. Along with this, a summary of the required capacity of the utilities used in the process is provided in Table 4 below.

Table 3: Utility Cost Summary		
Utilities Types	**$/Common Unit**	**$**
Steam		
High P	$/ 2,205 lbm	29.97
Med. P	$/ 2,205 lbm	29.59
Cooling Water	$ / 2,190,000 lbm	14.8
Process water	$/ 8.34 lbm	0.008
Thermal System		
90% Efficient	$/GJ	12.33
Electrical	$/ 1.343 hp*h	0.06
Tertiary Waste Water Treatment	$ / 2,190,000 lbm	56

Table 4: Utility Requirements and Yearly Cost for 100% Capacity		
Types/Location	**Capacity**	**Cost**
Steam from boilers	lbm/yr	$/year
high pressure / E-102	1.38E+08	$1,882,635
med pressure / E-100 and E-101	7.15E+07	$960,107
Cooling tower water	lbm/yr	
condenser-crystallizer	2.72E+10	$183,587
inside casting wheel	199728	$1
outside casting wheel	3.83E+07	$259
condenser-polymerization CSTR	5.02E+08	$3,393
condenser-casting wheel	6.25E+08	$4,227
Other Water	lbm/yr	
Process water / into Deionize tank	8.69E+08	$834,024
Thermal system	GJ/yr	
Dowtherm boiler / Polymerization CSTR	6.47E+03	$79,733
Electrical	hp.hr/yr	
pump / btw di water tanks	1.94E+04	$869
pump / to the crystallizer	2.23E+05	$9,976
pump / to polymerization CSTR	2.46E+04	$1,100
pump / to extruder	2.01E+05	$8,976
mixer / aq. HMDA tank	1.15E+04	$515
mixer / aq. adipic acid tank	7.63E+04	$3,409
agitation / aq. Nylon salt cstr	8.78E+04	$3,924
agitation / polymerization CSTR	2.01E+05	$8,982
drive / extruder	1.33E+05	$5,950
drive / casting wheel	8.37E+05	$37,408
drive / chopper	8.37E+05	$37,408
drive / dryer	1.00E+06	$44,882
drive / conveyer HMDA	1.45E+04	$647
drive / conveyer Adipic acid	1.58E+04	$707
	TOTAL COST	$4,139,141

Equipment List and Unit Descriptions

Pumps

There are a total of four pumps in the system, P-100, P-101, P-102, and P-103. The pressure of the streams entering and exiting the pumps were found by starting at a point where the pressure was known in the system, usually the design operating pressure of a connected piece of equipment before or after the pump of interest. All pumps in the process are centrifugal pumps, except for P-103, which is a reciprocating pump. P-103 is used in the process to pump the molten Nylon 6 6 product from the polymerization reactor to an extruder that operates at an extremely high pressure (1000 psia). Hence, P-103 was designed as a reciprocating pump in order to be able to handle such a large pressure increase. A summary of the pumps used in the system is provided in Table 5 below.

Table 5: Pumps in Process	
PFD Label	Description
P-100 A/B	Centrifugal pump between deionizers
P-101 A/B	Centrifugal pump between Nylon salt preparation reactor and evaporator
P-102 A/B	Centrifugal pump between crystallizer and polymerization reactor
P-103 A/B	Reciprocating pump between polymerization reactor and extruder

Heat Exchangers

Multiple heat exchangers were utilized in the process to either add heat to a process stream or to condense the steam that was produced by a process in the system. The key sizing parameter for a heat exchanger is the overall heat transfer area. The design equation to calculate the overall heat transfer area is shown in Equation 3 below [8].

$$A_o = \frac{q}{U_o \Delta T_{lm}} \quad (3)$$

Where:

A_o is the overall heat transfer area

q is the heat duty required

U_o is the overall heat transfer coefficient

$\Delta T_{lm}$is the log mean temperature

The heat duty can be estimated from the known conditions for each process stream, where the flowrate is known, using Equation 4 below.

$$q = \dot{m}C_p(T_{in} - T_{out}) \quad (4)$$

Where:

$\dot{m}$ is the mass flowrate of the considered stream

C_p is the specific heat capacity

T_{in} is the inlet temperature of the stream of interest

T_{out} is the outlet temperature of the stream of interest

Once this heat duty for the process stream is known, Equation 4 is then applied to the utility stream to calculate the mass flow rate of the desired utility.

Two heat exchangers in the process use medium pressure steam, including E-100 and E-101, to heat up process water prepared for the deionizer tower T-100 and the deionized water prepared for the mixing of adipic acid and HMDA solution. One heat exchanger, E-102, uses high pressure steam to add heat to the Nylon salt feed entering the crystallizer body. The saturated steam used in these three heat exchangers goes through a condensing process. Assuming the utility steam used is pure and the pressure drop is negligible, the condensation process can be estimated as an isothermal process. In order to account for phase change involved in the condensing process, latent heat of vaporization (h_{fg}') must be considered in the calculation of heat duty. Hence, the following equation must be utilized to calculate the required saturated steam utilities instead of Equation 4 above.

$$q = \dot{m}\, h_{fg}' \quad (5)$$

Three condensers were used (E-103, E-104 and E-105) to condense the water vapor produced by the process. Similar strategies of sizing a heat exchanger discussed above were applied for the sizing and costing of the condensers. A heuristic value of 150 Btu/hr.ft^2.°F was assumed for the overall heat transfer coefficient in all heat exchanger design since the process of condensing steam was involved in each heat exchangers [2].

The design operating pressure of each heat exchanger was the bubble point pressure at the considered steam temperature for the steam to be at its saturated condition. Only in the case where the condenser is used to cool the water vapor out the of the polymerization reactor, E-104, was the pressure of the reactor given priority. Hence, the operating pressure was calculated based on the design operating pressure of the reactor by assuming a 2 psi pressure drop in the return line from the reactor. A summary of the heat exchangers used in the system is provided in *Table 6* on the following page.

Table 6: Heat Exchangers in Process	
PFD Label	Description

E-100	Fixed Tube Heat Exchanger
E-101	Fixed Tube Heat Exchanger
E-102	Fixed Tube Heat Exchanger
E-103	Fixed Tube Heat Exchanger
E-104	Double Pipe Heat Exchanger
E-105	Diphenyl Heater

Deionized Water System

Deionized water was chosen for this system since it has lower operating costs than other water purification options. The deionized water system consists of two mixed-bed deionizers in series. The two deionizers both have a cation and anion resin. The resins consist of 40% hydrogen (cation) and 60% chloride (anion). Mixed-bed deionizers offer the desired pH and purity that is necessary for a polymer producing process. The pump between the two (P-100 A/B) mixed-bed deionizers is used to overcome the hydrostatic head between the first deionizer and the second deionizer. A pressure drop of 5 psi was assumed across each tower [2]. A mixed-bed deionizer was chosen in order to completely purify the water used for the solutions of HMDA and adipic acid that will be further processed into Nylon 6,6 [9]. The deionized water system equipment is listed in *Table 7* with the PFD Labels.

Table 7: Deionized Water System	
PFD Label	Description
T-100	Mixed Bed Deionizer with Chloride and Hydrogen Resin
T-101	Mixed Bed Deionizer with Chloride and Hydrogen Resin

Dry Storage System

It was determined that adipic acid and HMDA are crystalline solids at room temperature [10]. Also, since the reaction was chosen to run continuously, it is necessary to have bulk storage tanks within the plant to hold these raw materials, TK-100 and TK-102. It was determined that a maximum of six days, or close to one week, of solids needed to keep the process continuous would be stored in bulk on the plant. The storage was limited to six days in order to minimize the amount of HMDA needed to be stored under hygroscopic conditions [4]. This also helped to minimize the capital investment of the plant. Along with this, the six day time period of storage was justified as being large enough to keep the system running continuously for times when inclement weather or natural disasters are expected to delay delivery of raw materials to the plant. Shipments of both adipic acid and HMDA should be scheduled to be delivered every four days, leaving an amount of two days of raw material in the storage tanks before each delivery [2]. The specific diameter and length of these bulk storage tanks were determined by taking the volume needed for six days of solid storage and finding them such that L/D is close to 4. These storage tanks are vertical on concrete pads due to the capacity being greater than 10,000 gallons [2]. The storage tank for HMDA (ρ equal to 0.89 g/cm^3) is larger than for adipic acid (ρ equal to 1.366 g/cm^3) due to its lower density [5, 11]. Carbon steel was selected for TK-100 because adipic acid is compatible with carbon steel with only slight corrosion [12]. On the other hand, HMDA requires being stored in a tank with a phenolic lining due to its need for hygroscopic conditions [13]. Carbon steel was selected for this storage tank, TK-

102, as well due to this resin limiting the effect of HMDA on its environment. In addition, this tank requires storage under a nitrogen blanket to limit moisture from entering the storage tank and affecting the quality of the raw material [14]. The detailed calculations for sizing and costing these equipment, TK-100 and TK-102, can be found in Table A.5 and A.6 in the *Appendix* of this report.

Hoppers are the most common way to transport solids within a process to a mixer or reactor [15]. It was determined that two hoppers are necessary in the process of producing Nylon 6 6, TK 101 and TK-103, for controlling the mass of solid adipic acid and HMDA that will be added to two mixers with deionized water. Due to the typical hold-up time of hoppers being from one to three hours, a mid-range value of two hours was selected [15]. This hold-up time of two hours helps to further justify the need for the bulk storage tanks as opposed to single means of storage for each of the two solid raw materials. These hoppers were treated as vertical cylindrical storage tanks for the purposes of this preliminary design and were sized with an L/D factor equal to four. However, further detail needs to be taken to determine qualities of the hopper, such as the configuration and the outlet feeder, which will provide for a constant mass flow out of the hopper [15]. These parameters will also help to limit dead zones within the hopper where solid material does not flow. Another important way to limit dead zones within the hoppers is to keep the ambient temperature below the melting temperature of the solids. Adipic acid has a melting point of 304°F to 309°F, thus this is not a case for concern [5]. However, HMDA has a melting point of 108°F to 113°F [4]. The record high of the ambient temperature in Calvert City, KY is just below this melting temperature [16]. Thus, methods of cooling the hopper and bulk storage tank of HMDA should be investigated during detailed design to determine whether or not they are necessary. The detailed calculations for sizing and costing these equipment, TK-101 and TK-103, can be found in Tables A.9 and A.10 in the Appendix Section of this report.

In addition, screw conveyors were chosen to move the bulk solids into the system. These types of conveyors provide the power necessary to transport adipic acid and HMDA while also having the ability to be completely enclosed. This is an important factor when dealing with these chemicals which are toxic and corrosive. HMDA also needs to be protected from the atmosphere because it is hygroscopic. The specifications for design were determined from a design guide by Conveyor and Manufacturing Company. The capacity required corresponds to a screw diameter of six inches. In order to ensure that the screw conveyor will transport the materials at the rate expected, it is necessary to set the angle at or less than 15 degrees above the ground. The length of the conveyor is based on the maximum angle of 15 degrees, and estimating how high the material would need to be transported based on the height of the hopper. The drive power was sized based on the density and flow rate of the material as well as accounting for the angle of elevation. The detailed calculations for sizing and costing these equipment, MP-100 and MP-101, can be found in Tables A.7 and A.8 in the Appendix Section of this report. *Table 8* on the following page shows the list of equipment involved in this system.

Table 8: Storage Tanks of HMDA and Adipic Acid	
PFD Label	Description

TK-100	Adipic Acid Dry Storage Tank
TK-101	Adipic Acid Hopper
TK-102	HMDA Dry Storage Tank
TK-103	HMDA Hopper
MP-100	Screw conveyor to deliver Adipic Acid to M-100
MP-101	Screw Conveyor to deliver HMDA to M-101

Mixers

The two mixers used in this system, M-100 and M-101, are utilized to dissolve the adipic acid and HMDA solids in the system before they are mixed in the Nylon salt formation reactor. The key parameter used in sizing these mixer type reactors was the solubility of the raw materials. Adipic acid has a solubility in water of about 23 g per liter of water at 77°F [5]. It is crucial in this process to drive the solubility of adipic acid in water further by increasing the temperature of the water because this results in a smaller amount of deionized water needed in the process. This also causes the equipment further on in the process to be smaller because less water is required to be removed in the Nylon salt crystallizer. Thus, the deionized water is heated to 50°C or 122°F, at which the solubility of adipic acid in water is about 82.7 g in 1 L of water [17]. However, the amount of adipic acid added in the mixer, M-100, is limited to 90% of this maximum solubility, or 74.4 grams per liter of water to ensure proper dissolving of the solid. HMDA, on the other hand, has a relatively high solubility compared to adipic acid, at 637 at 20°C or 68°F [18]. Thus, the mixer used for this solution, M-101, was sized to be much smaller than that for the adipic acid. Due to a lack of solubility data for HMDA at 122°F, it was assumed that at least 637 g of it would be fully soluble in water at this temperature, hence this is what was used in calculating the volume of the reactor. A typical residence time of 30 minutes was selected for sizing calculations of these two mixers [19]. The final parameter needed to size these mixers was the mass flow rate of solids required for the polymerization reaction. Once this was determined from the Polymath calculations (see Figure A.1 in Appendix), and along with the solubility ratio of the solids to deionized water and the density of these solids, the volume of fluid within the mixers was calculated. This volume was then doubled to allow for half of the mixer volume to be used for liquid holdup [2]. The diameter and length of these mixers were then calculated based on the assumption that the L/D factor should be equal to two [2]. Both of these mixers were costed based on the information in Analysis, Synthesis and Design of Chemical Processes for carbon steel construction [2]. The operating cost for these mixers was found from the electricity needed for the drives of the mixers at their given capacities. The detailed calculations for sizing and costing these equipment, M-100 and M-101, can be found in Tables A.11 and A.12 in the Appendix Section of this report.

Table 9: HMDA and Adipic Acid Solution Mixers	
PFD Label	Description
M-100	Deionized water and Adipic Acid Mixer
M-101	Deionized water and HMDA Mixer

Nylon Salt Preparation Reactor

The Nylon salt solution producing reactor, R-100, was sized on the same principles as the adipic acid and HMDA mixers that feed to it. The total volumetric flow rate in is equal to the sum of the volumetric flow rates out of M-100 and M-101. It was assumed that the kinetics of this reaction could be simplified to instantaneous formation of the Nylon salt because the adipic acid and HMDA are already dissociated into the positive and negative ions before entering R-100. Thus, the reactor was treated as the mixers and a residence time of 30 minutes was assumed with a holdup time of 30 minutes as well. The required volume of the agitated reactor is outside of the costing correlations used from Analysis, Synthesis and Design of Chemical Processes. This is due to the large quantity of water required to dissolve the solid adipic acid in the prior mixer, M-100. A jacket is provided on this reactor in the case of needed cooling water to cool the mixing reaction [20]. The operating cost for this agitated reactor was found from the electricity needed for the drive at its given capacity. The detailed calculations for sizing and costing of this piece of equipment, R-100, can be found in Table A.13 in the Appendix Section of this report.

Table 10: Nylon Salt Preparation Reactor	
PFD Label	Description
R-100	Reactor to produce Nylon Salt

Evaporative Crystallizer System

The main objective for the utilization of a crystallizer in the system was to prepare Nylon salt from an equimolar aqueous solution of adipic acid and HMDA to proceed into the polymerization CSTR. The technique of crystallization for separation of the Nylon salt and water is more suitable for this project over other separation techniques due to a significant difference in melting point between water (0°C) and Nylon 6 6 salt (190°C) [21].The crystallization was designed to be carried out on a continuous basis. Most process plants favor continuous equipment due to the fact that the operating conditions are adjustable, less operating labor force is required, and usually, the process is more economical in terms of overall energy use and product characteristics [22]. The type of crystallizer chosen was the forced-circulation crystallizer functioning as an evaporative crystallizer (also known as a forced-circulation evaporator). Besides the fact that forced-circulation evaporator is widely used in the industry and is normally a less expensive type of separation equipment available, other characteristics of this specific type of crystallizer were considered to better support the process of this project. These characteristics include its probability to handle a large rate of evaporation and solutions with high viscosity. It is also favorably used for when an intermediate is formed [23]. The aqueous Nylon salt solution that leaves the reactor R-100 can be considered an intermediate product of adipic acid and HMDA.

The equipment design of the crystallizer starts with the feed of aqueous Nylon salt solution coming from the mixer. This feed first passes through a circulation pump and is heated in a heat exchanger before entering the crystallizer body. Evaporation of the water solvent occurs at the top surface of the salt slurry, while nucleation takes place near the bottom of the crystallizer body. The Nylon salt crystals then are removed from the bottom of the equipment while the water vapor goes through a condenser out the top of the crystallizer. The forced-circulation evaporator design procedure involved the sizing of crystallizer body, a heat exchanger to add heat to the incoming feed, and a condenser for the water evaporating and being removed out of the top of the crystallizer body. A summary of the equipment involved in the crystallizer is detailed below in *Table 11*.

Table 11: Crystallizer	
PFD Label	Description
R-101	Evaporator Crystallizer
E-102	Fixed-Tube Heat Exchanger
E-103	Condenser

The key design variable in sizing the crystallizer body is the maximum vapor velocity of the water solvent in the Nylon salt solution. The maximum vapor velocity was calculated using the following equation:

$$V_{max} = C_v(\frac{D_l - D_g}{D_g})^{1/2} \tag{6}$$

Where:

Vmax is the maximum vapor velocity of the vapor leaving the liquid surface of the salt solution

D_l is the liquid density of the solvent

D_g is the vapor density of the solvent

C_v is a constant depending on loading, pressure, and allowable entrainment.

A C_v value of 0.08 ft/s is found and recommended for vapor pressure [22]. Since the key capacity parameter for costing the forced-circulation evaporator is the cross-sectional area of the crystallizer body [2]. The required minimum design of cross-sectional area must be able to handle the vapor traffic across the top portion of the crystallizer. An estimated value of 9 ft was used as the starting point for the diameter for the crystallizer body. The value of diameter was varied and adjusted until the cross-sectional area satisfied the expectation of handling the water vapor load.

According to the heuristic of sizing a crystallizer, the operating condition is suggested to be about equal to the melting (freezing) temperature of the solute [23]. Melting temperature of Nylon salt is found from literature to be approximately at 374°F [24]. The overhead pressure of the crystallizer body can be estimated via the bubble point calculation of the water in the condenser (E-104). Since the evaporative crystallization can generally be done at a constant temperature condition, the water that evaporates out of the top of the crystallizer body and goes through the condenser is assumed to have the same temperature as the process occurring inside the crystallizer body, which is at 374°F.The bubble point pressure at 374°F was then determined for the water vapor in the condenser. Assuming a 2 psi pressure drop through the returning line, the pressure of the overhead crystallizer body was then calculated.

Polymerization Reactor

The role of a reaction vessel in this system is to carry out the polycondensation reaction of the hexamethylenediammonium (Nylon 6 6 salt) to produce Nylon 6 6. Hence, the polymerization reactor should be considered the most important piece of equipment and its design and costing was given priority within this project. Sizing the reactor for the polymerization of Nylon 6 6 depended on the type of reactor, space time, and chemical kinetics for the polymerization of Nylon 6 6. The design pressure and temperature required to create the most desirable reaction conditions were also accounted for. The objective of the reactor design was to meet the required product rate specification of 85 MMlbs per year of nylon 6 6 and to achieve a high-quality nylon 6 6 product (high number-average degree of polymerization and molecular weight). The design operating pressure and reaction temperature should be optimized within the scope of process safety and environment. *Table 12* summarizes the equipment required for the polymerization reactor system of the process. A detailed explanation of the design methodology follows.

Table 12: Polymerization Reactor	
PFD Label	Description
R-102	Polymerization Reactor
E-104	Double Pipe Heat Exchanger
E-105	Fixed Tube Heat Exchanger

A continuous-stirred-tank reactor (CSTR) was chosen in this project to carry out the polymerization process to produce molten Nylon 6 6. Some of the characteristics and advantages of a CSTR were considered to support the choice of it as a polymerization reactor including: [25], [1] and [26.]

- Economical and widely used for high-capacity plants while batch reactors are known particularly for low production capacities
- Well-mixed conditions can help prevent problems when the polymers produced become viscous, which would not be mitigated by a plug-flow-reactor (PFR)
- Mixing enhances the heat transfer characteristics and creates easier temperature control by helping to avoid hot spots
- The water solvent and water by-product in the polymerization reaction can be boiled to remove the heat of polymerization
- Constant copolymer composition can be achieved in a CSTR while a varied composition mixture might be produced by PFRs or batch reactors

Since the residence time distribution is wide for CSTRs, one well-known disadvantage when using this type of reactor is that a high conversion will be difficult to attain. However, in a step-growth polymerization, the conversion of monomer does not indicate much about the yield of the desired polymer. This is due to the fact that it is the functional reactive end-groups from each end of the monomers that react with each other. Thus, the reaction will still proceed even when all the monomers have been consumed because it is the end groups that are reactive [27].

A chemical reaction algorithm was developed in this project to study several variables in the system. These include space time, design temperature of the incoming feeds, heat transfer fluid used, reactor volume, the mass flow rate of the incoming feed, as well as the reaction temperature. The step-by-step algorithm model equations described below were solved using the computation software, Polymath. The kinetic parameters and rate law model were obtained based on Steppan's kinetic and equilibrium models for Nylon 6 6 polymerization [28].

Chemical Reaction Engineering Algorithm Model for Nylon 6 6 Polymerization in a CSTR

[28], [29] and [30]

1. Chemical Reactions Conventions:

$$a + c \leftrightarrows l + w \tag{7}$$

Where:

a is amine end-group (-NH2)
c is carbonxyl end-group (-COOH)
l is the amide linkage
w is the water molecule

2. Design Specification and Initial Condition:

$$F_l = \frac{(85E6\ lbm/year)}{(365\ days/year) * (24\ hours/day) * (service\ factor)} \tag{8}$$

Where:

$\tau = 5\ hours$
$T_o = 190\ °\text{C} = 374\ °\text{F}$
$T_a = 300\ °\text{C} = 572\ °\text{F}$

3. Mole Balance for CSTR:

$$V = \frac{F_{ao} - F_a}{-r_a} \tag{9}$$

$$V = \frac{F_{co} - F_c}{-r_c} \tag{10}$$

$$V = \frac{F_{lo} - F_l}{-r_l} \tag{11}$$

$$V = \frac{F_{wo} - F_w}{-r_w} \tag{12}$$

4. Rates Law:

$$r_W = C_T * \frac{k}{3600} * (x_a x_c - x_l x_w / K) \tag{13}$$

$$k = k_o * exp(\left(\frac{E}{R} * \left(\frac{1}{T_r} - \frac{1}{T} \right) \right) \tag{14}$$

$$K = K_o * \exp \left(\Delta H_o * \frac{10^{-3}}{R} * \left(\frac{1}{T_r} - \frac{1}{T} \right) \right) \tag{15}$$

$$k_o = exp \left(2.55 - 0.45 \, tanh\big(25(x_w - 0.55)\big) \right) + 8.58 \, tanh\big(50(x_w - 0.10)\big) - 1)(1 - 30.05 x_c) \tag{16}$$

$$K_o = exp(1 - 0.47 * exp \left(-\frac{\sqrt{x_w}}{0.2} \right) * (8.45 - 4.2 x_w)) \tag{17}$$

$$\Delta H_o = 7650 \, tanh\big(6.5 * (x_w - 0.52)\big) + 6500 \, exp \left(-\frac{x_w}{0.065} \right) - 800 \tag{18}$$

$T_r = 200\ ℃ = 392\ ℉$

$E = 21.4 \frac{kcal}{mol}$

$R = 0.001987\ kcal/mol.K$

5. Stoichiometry:

$$C_t = C_a + C_c + C_l + C_w \tag{19}$$

$$x_a = \frac{C_a}{C_t} \tag{20}$$

$$x_c = \frac{C_c}{C_t} \tag{21}$$

$$x_l = \frac{C_l}{C_t} \tag{22}$$

$$x_w = \frac{C_w}{C_t} \tag{23}$$

$$F_a = C_a * v_o \tag{24}$$

$$F_c = C_c * v_o \tag{25}$$

$$F_l = C_l * v_o \tag{26}$$

$$F_w = C_w * v_o \tag{27}$$

$$v_o = \frac{V}{\tau} \tag{28}$$

6. Energy Balance:

$$UA(T_a - T) - F_{ao}(Cp_a + Cp_c)(T - T_o) + V\Delta H_{rxn} r_w = 0 \quad (29)$$

$$\Delta H_{rxn} = 4.184\,\Delta H_o + (Cp_l + Cp_w - Cp_a - Cp_c)(T - T_r) \quad (30)$$

$$Cp_a = 68.14\,\frac{J}{mol}.K$$

$$Cp_c = 275.37\,\frac{J}{mol}.K$$

$$Cp_l = 377.92\,\frac{J}{mol}.K$$

$$Cp_w = 75.4\,\frac{J}{mol}.K$$

The Polymath coding and reports are provided in Figure A.1 in the Appendix section of this report. For the purposes of clarity, Table 12 has been provided on the following page to define the variables and their meaning within the CRE Algorithm.

Table 13: Nomenclature used in the CRE Algorithm			
Term	**Definition**	**Unit**	**Source**
F_{io}	Initial molar flowrate of species i	mol/s	
F_i	Molar flowrate of species i	mol/s	
C_{io}	Initial concentration of species i	mol/m^3	
C_i	Concentration of species i	mol/m^3	
C_t	Total concentration	mol/m^3	
r_i	Reaction rate for component i	mol/m^3.s	
x_i	Mole fraction of component i	mol/mol	
T_o	Initial temperature	Kelvin	[31]
T_a	Medium fluid, Dowtherm, temperature	Kelvin	[2]
T_r	Referenced (ref.) temperature	Kelvin	[28]
T	Reaction temperature	Kelvin	
k_o	Rate constant at ref. temperature	hr $^{-1}$	[28]
K_o	Equilibrium constant at ref. temperature		[28]
k	Rate constant	hr $^{-1}$	[28]
K	Equilibrium constant		[28]
E	Activation energy	kcal/mol	[29]
R	Ideal gas constant	kcal/mol.K	
ΔH_o	Heat of reaction at ref. temperature	cal/mol	[28]
ΔH_{rxn}	Heat of reaction	J/mol	
τ	Residence time, or space time	second	[29]
V	Liquid volume in the reactor	m^3	
v_o	Space time velocity	m^3/s	
U	Overall heat transfer coefficient	W/m^2.K	[2]
A	Reactor heat-exchange area	m^2	
Cp_i	Heat capacity	J/mol.K	

The polycondensation of nylon 6 6 salt can be carried out at high temperature (392°F -509°F) and high pressure (213-284 psi) [29] and [24] and [32] and [3]. Also, it was desired to maintain the reaction temperature below the degradation temperature of the reaction components. This is especially important for the adipic acid and Nylon 6 6, whose melting temperatures are approximately 554°F.

The reaction temperature was adjusted by varying the initial temperature of the incoming feeds (stoichiometric equivalent nylon salt slurries), and the initial temperature of the heat exchange fluid (Dowtherm flowing through the reactor's jacket). The Nylon salt feed that comes in to the polymerization reactor is prepared from the evaporative crystallizer, which is set to operate at the melting point temperature of Nylon 6 6 salt. Hence, melting point of Nylon 6 6 salt, which is at 374°F, should be an appropriate starting point to specify the feed temperature. Considering that monomers and polymers are poor conductors of heat [3] and also that the reaction is endothermic at water compositions greater than 52 mol % [28], heat has to be added to the reaction via a Dowtherm jacket. This is necessary to increase the rate of reaction to a greater value. It was desirable for the reaction temperature to be at the higher end of the temperature range in order to increase the reaction rates, but not so high that the reaction components start to degrade. This degradation produces carbon dioxide (CO_2) [30], and should be monitored to avoid unsafe reaction conditions.

Considering that the condensation of Nylon salt proceeds only if the by-product water is removed, the operating pressure, was decided such that at the determined reaction temperature, water will vaporize and be removed from the reactor. The design pressure must be lower than or equal to the vapor pressure of water at the reaction temperature. The design operating pressure of 250 psi was decided due to the findings from a more recent source [24] for the process pressure of polymerization to produce Nylon 6 6, which satisfied the design expectations for operating pressure.

Table 14: Chemical Kinetic Results	
Flowrate and Reaction Rate of each Components	**Value**
F_{ao}, mol/s	6.21
F_{co}, mol/s	6.21
F_{lo}, mol/s	0
F_{wo}, mol/s	6.21
F_a, mol/s	0.52
F_c, mol/s	0.52
F_l, mol/s	5.69
F_w, mol/s	11.90
r_a , mol/m^3.s	0.22
r_c , mol/m^3.s	0.22
r_l , mol/m^3.s	-0.22
r_w, mol/m^3.s	-0.22

Table 15: Desired Product (Nylon 6 6) Quality	
Quality	**Value**
Instantaneous Yield	1
Overall Yield	1.00
Number-average degree of polymerization	11.87
Number-average molecular weight (g/mol)	2687.02

Table 16 : Polymerization CSTR Equipment Design Specification		
Sizing Parameter	**Value**	**Justification**
Reactor volume, ft3	780	
Space time, hours	5	Reaction reaches equilibrium after 5 hours [29]
Liquid Level, ft	8	
Diameter, ft	8	Heuristic for reactor: liquid level equals diameter [2]
Height, ft	15.5	Assuming the height is double the liquid level
Wall thickness, ft	1.5	Heuristic for reactor: less than ¼ of diameter [2]
MOC	Stainless Steel	Due to the acid component (Adipic acid)
Process Conditions	**Value**	**Justification**
Temperature, °F	515	[Polymath]
Operating pressure, psia	250	[28] and [29]

Mechanical Processing

Extruder

After exiting the polymerization reactor, the molten Nylon passes through a reciprocating pump to increase the pressure significantly. The reciprocating pump is necessary in order to allow for such a large pressure change. Reciprocating pumps work well for medium capacities and clean liquids. The molten Nylon then enters a single-screw, rapid compression extruder. The extruder consists of three sections, feed, compression, and metering. Due to the high viscosity of Nylon 6, 6, the polymer should be compressed quickly in order to avoid plugging within the extruder. High pressures are used within the extruder to ensure that the molten Nylon is compressed for the casting wheel system [33]. The exiting Nylon from the extruder is still molten, but now it is in thinner strand to be cooled down and solidified during the next mechanical processing step. The extruder requires a drive in order to operate at these conditions [34].

Casting Wheel

The casting wheel spins the molten Nylon strands on a wheel in order to prepare sheets to be chopped. The Nylon is sprayed with cooling water that immediately vaporizes because of the high temperature of the material at the extruder outlet. The Nylon solidifies due to this cooling process. The steam is treated and recycled using a condenser in order to minimize operating costs. The casting wheel is kept near a constant pressure because of the condenser. It will be in a place of limited traffic to avoid anyone being exposed to the high temperatures [35]. The casting wheel is powered by a drive that allows the wheel to turn at a constant speed in order to properly form the Nylon sheets. The casting wheel drum is also cooled from the inside to avoid overheating of the wheel. The amount of cooling water necessary was based on conduction heat transfer. The drum is hollow, so process water can flow through in order to ensure that the equipment exhibits minimal temperature change and damage.

Chopper

The sheets of solidified Nylon pass through a chopper that cuts the Nylon sheets into granules that will be further processed and sold to the specified customer. The chopper is powered by a drive in order to reach the necessary constant cutting speed [36]. The pressure and temperature remain constant during this process since it is a quick procedure.

Dryer

A continuous vacuum drum dryer is used to completely dry the granules. This is an important step in order to ensure that there is a minimal amount of moisture in the granules. A significant moisture level will degrade the Nylon over time, so a lengthy drying time is necessary. The granules will be dried for ten hours, and then the temperature of the granules will be reduced before entering the storage container to avoid degradation. The granules are dried by using steam that passes through the jacket of the dryer. The dryer is also agitated in order to ensure consistent drying of all the granules. The dryer is powered by a drive. Dryers generally exhibit a pressure drop of 5 psi during this process [37].

Nylon Granule Storage Hopper

The dried granules are stored in a hopper to allow for quick delivery to trucks. The storage hopper was sized to hold four days' worth of pellets. The inventory is kept low in order to allow for quick turnover of the product. The hopper is made of carbon steel and is kept at a constant temperature of 158 °F to ensure the granules keep the optimum properties of Nylon. The hopper will be enclosed to ensure water moisture remains out of the granules.

Table 17: Mechanical Processing Equipment	
PFD Label	**Description**
P-103 A/B	Reciprocating pump between polymerization reactor and extruder
MP-102	Single-screw, rapid compression extruder
MP-103	Casting wheel
E-105	Condenser for steam condensate leaving the casting wheel
MP-104	Chopper
MP-105	Vacuum, Paddle Drum Dryer
TK-104	Storage Hopper for Nylon granules

Equipment Specification Sheet

Table 18: Equipment Summary for Nylon 6 6 Manufacturing							
Tanks/Towers	TK-100	TK-101	TK-102	TK-103	TK-104	T-100	T-101
Volume (ft3)	12164	344	14867	424	13784	177	177
Temperature (oF)	70	70	70	70	158	100.4	100.4
Pressure (psia)	14.7	14.7	14.7	14.7	9.7	100	100
Orientation	Vertical	vertical	vertical	vertical	vertical	vertical	vertical
Height/Length (ft)	60.5	17.5	65.5	15	65.5	9	9
Diameter (ft)	16	5	17	6	16.5	5	5
MOC	CS	CS	CS	CS	CS	CS	CS
Mixers/Reactors	M-100	M-101	R-100	R-101	R-102		
Type	reactive	reactive	jackt.ag.	FCP	jackt.ag.		
Volume (ft3)	1645	249	1901	1438	780		
Temperature (oF)	122	122	122	374	515		
Pressure (psia)	90	90	90	183.4	250		
Orientation	Vertical	vertical	vertical	vertical	vertical		
Height/Length (ft)	19	10.5	20	14	8		
Diameter (ft)	10.5	5.5	11	11	15.5		
MOC	CS	CS	CS	SS	SS		
Heat Exchangers	E-100	E-101	E-102	E-103	E-104	E-105	
Type	fixed tube	fixed tube	fixed tube	fixed tube	double pipe	fixed tube	
Area (ft2)	337	170	373	2142	31	121	
Duty (BTU/hr)	5.06E+06	2.26E+06	1.21E+07	8.81E+07	1.63E+06	2.03E+06	
Tube Temp In/Out (oF)	377/377	377/377	122/374	86/113	86/113	86/113	
Tube Pressure (psia)	189.7	189.7	196	100	100	100	
Tube Phase	condensing	condensing	liq./precip.	liquid	liquid	liquid	
Tube MOC	CS	CS	SS	SS	SS	SS	
Shell Temp In/Out (oF)	52/100.4	100.4/122	489/489	374/374	515/400	212/212	
Shell Pressure (psia)	105	95	614.7	181.4	250	14.7	
Shell Phase	Liquid	liquid	condensing	condensing	condensing	condensing	
Shell MOC	CS	CS	CS	SS	SS	SS	
Pumps	P-100 (A/B)	P-101 (A/B)	P-102 (A/B)	P-103 (A/B)	***Heaters***		H-100
Type	Centrifugal	centrifugal	centrifugal	reciprocating	Type		diphenyl
Capacity (gpm)	210.1	195.25	27.23	19.8	Dowtherm Pressure (psi)		152.7
Fluid Density (lbm/ft3)	62	74.96	63.24	71.17	DowthermTemperature (°F)		572
Temperature (oF)	100	122	374	515	Duty (MJ/hr)		780
Psuction (psi)	95	90	189	250	MOC		N/A
Pdischarge (psi)	104	196	259	1002			
Shaft Power (hp)	2.1	23.7	2.74	21.72			
Efficiency of drive (%)	90	90	90	90			
MOC	SS	SS	SS	SS			
Mechanical Processing	MP-100	MP-101	MP-102	MP-103	MP-104	MP-105	
Type	screw conveyor	screw conveyor	extruder	casting Wheel	chopper	dryer	
Drive (kW)	1.41	1.03	12	75	75	90	
Height/Length (ft)	62	62	20	5	3	20	
Diameter (ft)	1/2	1/2	2/3	16.5	5	7.5	
MOC	N/A	N/A	CS	SS clad	N/A	N/A	

Key:	
liq.	liquid
precip.	precipatate
FCP	Forced circulation (pumped)
Jackt.Ag.	Jacketed agitated
Cross.	cross-sectional

Equipment Cost Summary

Table 19: Equipment Cost Summary				
Equipment List	**PFD Label**	**Type**	**Price- Cbm (2016)**	**Source**
Adipic Acid Bulk Storage	TK-100	Vertical Process Vessel	$ 1,545,086	[2]
Adipic Acid Hopper	TK-101	Vertical Process Vessel	$ 48,695	[2]
HMDA Bulk Storage	TK-102	Vertical Process Vessel	$ 1,961,037	[2]
HMDA Hopper	TK-103	Vertical Process Vessel	$ 59,721	[2]
Nylon 6 6 Storage	TK-104	Vertical Process Vessel	$ 2,288,822	[2]
Deionizers	T-100 / T-101	Vertical Process Vessel	$ 99,301	[2]
Adipic Acid Mixer	M-100	Reactor- Mixer	$ 1,573,277	[2]
HMDA Mixer	M-101	Reactor- Mixer	$ 674,610	[2]
Nylon Salt Mixer	R-100	Reactor- Jacketed Agitated	$ 577,356	[2]
Evaporator/Crystallizer	R-101	Crystallizer with HEX	$ 1,406,576	[2]
Polymerization CSTR	R-102	Reactor- Jacketed Agitated	$ 722,962	[2]
Process Water HEX	E-100	Fixed Tube	$ 78,949	[2]
Deionized Water HEX	E-101	Fixed Tube	$ 71,540	[2]
HEX of Feed to Crystallizer	E-102	Fixed Tube	$ 125,633	[2]
Condenser for Steam out of Crystallizer	E-103	Fixed Tube	$ 269,009	[2]
Condenser of Steam out of CSTR	E-104	Double Pipe	$ 23,120	[2]
Condenser of Steam out of Casting Wheel	E-105	Fixed Tube	$ 130,804	[2]
Dowtherm Boiler	H-100	Diphenyl Heater	$ 60,755	[2]
Pump to Deionizer T-101	P-100 (A/B)	Centrifugal	$ 19,375	[2]
Pump to Crystallizer	P-101 (A/B)	Centrifugal	$ 48,894	[2]
Pump to Polymerization	P-102 (A/B)	Centrifugal	$ 49,123	[2]
Pump to Extruder	P-103 (A/B)	Reciprocating	$ 271,743	[2]
Screw Conveyor- AA	MP-100	Screw Conveyor	$ 16,934	[2]
Screw Conveyor- HMDA	MP-101	Screw Conveyor	$ 16,890	[2]
Extruder	MP-102	Extruder	$ 61,131	[23]
Casting Wheel	MP-103	Horizontal Process Vessel	$ 406,115	[2]
Cutter/Chopper	MP-104	Blender	$ 241,987	[2]
Dryer	MP-105	Dryer-Drum	$ 155,087	[2]
			$ 13,004,532	Fixed Capital Cost

Fixed Capital Investment Summary

The fixed capital investment begins by determining the cost of the individual pieces of equipment in the process. Most of the equipment was costed by the method in Turton. This begins by using the following equation:

$$log_{10}C_p^o = K_1 + K_2 log_{10}(A) + K_3[log_{10}(A)]^2 \quad (31)$$

Where:

$C_p^o = purchased\ cost$

K_X= Constants specific to each equipment type

A = Capacity of equipment

If the equipment type was not explicitly listed in the tables, then a comparable type of equipment was used to provide the K values. The equipment list includes a description of the actual function of the equipment as well as the equipment type used in the costing tables. Drives were costed and added to the pieces of equipment where necessary. Each pump cost includes the price of a spare pump. After the purchased cost is calculated, it can be adjusted to the bare module cost. This cost accounts for the pressure and material of construction.

The costing of the extruder for polymers was determined from a scale up procedure outlined in Rule of Thumb in Engineering Practice [23].The free-on-board cost (FOB) for a smaller extruder was given, and this value was scaled up based on the power required for the drive (*Table A.23* in the *Appendix*). The parameters used to determine the bare module cost of the extruder are available in *Table 20* below. First, the FOB value for the extruder provided was scaled up to be used for a 12 kW drive as opposed to the 10 kW drive provided. Then, using equation # through #, the bare module cost can be calculated for a carbon steel extruder. The percentages in equation # and # for the FOB cost were estimations based on instrumentation, infrastructure, taxes, and insurance costs factored in to the bare module cost [23].

Table 20: Parameters used for Extruder Costing

Costing Parameter	**Description**
FOB	Free-on-board cost
n	Scale up factor
L+M*	Free-on-board, cost for carbon steel factor
L+M cost	Accounts for instrumentation material and labor costs
PM	Physical Module Cost
BM	Bare Module Cost

The equations used for costing the extruder are listed below:

$$FOB_2 = FOB_{reference}(\frac{size_2}{size_{reference}})^n \quad (32)$$

$$L + M\ Cost\ =\ FOB\ \times\ L + M^* \quad (33)$$

$$PM = L + M\ cost\ + 0.2FOB \quad (34)$$

$$BM = PM +\ 0.1FOB \quad (35)$$

After all of the equipment costs were found the grassroots cost could be calculated. The grassroots cost was used to account for land and building development. It includes the total module cost which accounts for small alterations to existing plants.

$$C_{GR} = C_{TM} + 0.50 \sum_{i=1}^{n} C_{BM,i}^{o} \quad (36)$$

Where:

$$C_{TM} = total\ module\ cost$$

$$C_{BM,i}^{o} = bare\ module\ cost\ for\ base\ conditions$$

The total module cost is the bare module cost, contingency costs and fees. The textbook recommends using 15% and 3% of the bare module cost to account for contingency costs and fees, respectively. Next, this value can be added to the auxiliary facilities costs to account for the grassroots cost. Auxiliary facilities costs are calculated by taking 50% of the bare module cost. This percentage can generally range anywhere from 20% to 100%, however, 50% was assumed to be a conservative estimate and was used in this project. The grassroots costs represent the fixed capital for the project. The results of performing these calculations are summarized in *Table 21.*

Table 21: Fixed Capital Investment Summary	
Grassroots Cost - Fixed Capital Investment	$38,233,000
Total Module Cost	$15,345,000
Contingency Costs	$1,951,000
Fees	$390,000
Working Capital	$5,735,000
Cost of Manufacturing without depreciation (COM)	$153,600,000

Safety, Health, and Environmental Considerations

Safety

Inherent safety was addressed in this preliminary design by analyzing potential hazards before the plant design was implemented (*Table 22*). A major parameter considered in the polymer production process was the reaction chemistry. To avoid potential runaway reactions, cooling jackets were implemented as well as emergency cooling water systems within the control strategy. Working conditions within the plant for operators were also addressed to ensure that all employees will be able to operate equipment in a safe manner. Unsafe working conditions can be corrected by providing personal protective equipment for workers, limiting traffic near the dangerous equipment, and educating visitors and employees on how to operate the equipment on a daily basis, as well as in an emergency situation. Therefore, by determining and implementing a plan before the design is even implemented, the plant will be inherently safer.

A preliminary hazard and operability study was conducted in order to predict major potential hazards that could occur within the Nylon plant. The major concerns for this plant are runaway reactions, high temperatures, and high pressures within the equipment. These concerns will be addressed through the use of high pressure and temperature alarms and emergency shutoff systems (*Table 23*). All visitors and employees will be educated on how to respond to these emergency situations as well.

A preliminary hazard analysis was conducted in order to analyze the components through the process and how this would have a major impact on people in the plant, the major pieces of equipment, and the surrounding community (*Table 24*). The main concerns were with how to store and handle the components to ensure dangerous situations are avoided. HMDA, adipic acid, and nitrogen are chemicals that must be handled with care. The proper personal protective gear must be used when handling the components to ensure no improper exposure to the chemicals occurs.

These hazard and safety analyses were all conducted for a preliminary design. Before implementing the Nylon production process, it is recommended that other experienced and knowledgeable engineers and employees be included in the safety analysis process.

Table 22: Inherent Safety Table		
Hazard	**Inherent Safety Concept**	**Action**
Nylon Salt Reaction is exothermic	Attenuation or Moderation	Use a cooling jacket on reactor (control valve fails open)
		Further R&D to determine how exothermic the reaction is
Polymerization Reaction is endothermic when water content is more than 52 mol% [28]	Attenuation or Moderation	Have an emergency shutoff system of steam jacket if reactor gets too hot
		control valve fails open to release cooling water
		Temperature sensor
Cutting mill is very loud	Attenuation or Moderation	Provide appropriate hearing protection for all operators and visitors
		Limit traffic to cutting mill to only when necessary
HMDA is a toxic and hygroscopic component	Intensification or minimization	Purchase a certain amount of HMDA for a specified time to not have the chemical around for a long period of time
		Use nitrogen to preserve HMDA in storage container; keep moisture out
	Substitution	Corrosive to metal-Use phenolic resin to coat storage tanks to resist corrosion
		Use stirred tanks to decrease inventory of product as opposed to batch reactors
Waste water leaving evaporative crystallizer	Intensification or minimization	Needs to be treated to environmental standard in order to be disposed of in any body of water
		Nylon salt is dangerous to aquatic life, so water must be treated if small amount of Nylon salt is in the condensate
Adipic Acid	Intensification or minimization	Needs to be stored in a well vented area
		dangerous to aquatic life; proper disposal will be carried out
		can form combustible dust concentrations in air; keep in a well ventilated area
High pressure steam jacket to heat polymerization reaction	Substitution	Use a different material as opposed to high pressure steam such as Dowtherm
High temperature steam leaving the casting wheel	Attenuation or Moderation	control temperature
		Condense and reuse steam
High pressure leaving the extruder	Attenuation or Moderation	Use a reciprocating pump to handle large pressure drop

Table 23: Hazard and Operability Study

Guide Word	Deviation	Causes	Consequences	Actions
NO	No cooling	Cooling water fails to engage	Temperature will increase on R-100, E-103, E-104, MP-103, and E-105 due to the lack of heat removal cooling fluid	Have a high temperature alarm (TAH)
NO	No pumping	Pump malfunctions	Potential runaway reaction in R-102 if P-102 A/B fails	Have a high pressure alarm (PAH)
			More pressure in R-102 if P-103 A/B fails	
			Less pressure in MP-102 if P-103 A/B fails	
MORE	More steam	Control valve fails open	High temperature and pressure in E-102 and R-101 could cause unsafe conditions	Have a high temperature alarm (TAH)
MORE	More Heating	Temperature control fails	High temperature in H-100 lead to unsafe conditions and high temperature in R-102 could cause Nylon to degrade and release CO_2 as an undesired side product	Have a high temperature alarm (TAH)
				Emergency cooling water system available

Table 24: Hazard Analysis Table					
Process	**Hazard**	**Potential Causes**	**Major Effects**	**Hazard Category**	**Preventative Measures Suggested**
Adipic Acid Tank	Combustible Dust Formation	Transfer of Adipic Acid to storage container	Could ignite and cause a fire	1D	Keep adipic acid in a closed container and keep the vessels in a well-ventilated area, use of closed conveyor equipment
	Toxic when inhaled	Adipic Acid not stored or transferred properly	Toxic to visitors and employees if inhaled	2D	Keep permissible exposure limit of adipic acid under 5 mg/m^3 in the air
HMDA Tank	Can cause serious eye damage	Improper handling and storage	Loss of eye sight	2D	Use proper safety handling, and limit exposure by the storage and transportation equipment
	Chemical is dangerous if inhaled	improper storage	Difficulty breathing, toxic to visitors/employees	2D	Full face respirators required when in area that has an open container of HMDA; Keep permissible exposure limit to 2.3 mg/m^3
	Dangerous to environment	Improper Disposal	Damages to wildlife and water supply	2D	Disposal: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.
	Hygroscopic Material could degrade if not kept at proper conditions	Exposure to water or oxygen	Poor production, loss of profit	4C	Store under inert gas
	Further processing of solids can produce a combustible gas	Improper handling	Could ignite and cause a fire	2D	Provide appropriate ventilation where dust is formed, Firefighting Measures - Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide
Nitrogen Tank	Dangerous if inhaled	improper storage of nitrogen	Can cause asphyxiation	3E	keep in properly rated storage vessels and in a well-ventilated area;
Salt Formation Reactor	Exothermic Reaction occurs	Reactor could overheat and become over pressurized, explosion	Reactor becomes over pressurized or temperature increases too much	1E	Cooling jacket; fail open to allow for cooling water
Crystallizer	High pressure system	High pressure is necessary to the process	Evaporator could become over pressurized and cause an unsafe work environment, explosion	1D	Use steam to cool down the crystallizer and operate at a pressure that is as safe as possible given the conditions, use equipment and materials that are rated for high pressure
Polymerization Reactor	Reaction has potential to be exothermic	Not a high enough mole % of water entering the reactor	Runaway Reaction could occur	2D	Emergency shut down system that allows cooling water to cool down the reactor
	High temperature necessary for reaction to take place	Improper utility, improper reactor controls	Burns, unsafe pressures in reactor jacket, Nylon degrades and releases CO_2	3C	Use a Dowtherm jacket to heat reactor instead of high pressure steam, temperature control system
Extruder	Overheating of the screw	Operate at too high of a screw speed	Damage equipment and Nylon	4C	Operate extruder at a safe and constant speed
	Process malfunction, pressure/product build up	Nylon stays in extruder too long	Potential plugging in the extruder	3D	Avoid plugging in the extruder by cleaning with steam after shutdown
Chopper	Equipment produces excessive noise	Not properly contained	Can cause hearing damage to visitors and employees	4B	Hearing protection required and limit traffic near chopper
	Potential for cut material to escape the equipment	Cutting speed is too high, improper containment	Personal injury	3D	Cover chopper, require protective safety shields when person in the area
Casting Wheel	Steam from cooling water stream will be hot	water vaporizes when it touches the Nylon fibers	Burns	3D	Keep the casting wheel contained, use proper condenser, label hot streams
Dryer	Reaches high temperatures	Temperature of dryer not controlled properly	Nylon could degrade and temperature could be dangerous to operators	3B	Provide a jacket on the dryer and a temperature control system to maintain a safe temperature level in the system

Sustainability and Environmental Concerns

All wastewater used in the Nylon plant will be treated using the tertiary water treatment process [2]. Tertiary water treatment involves a filtration, activated sludge, and chemical processing procedure to ensure the water is not hazardous to the environment. The water produced by the process, cooling water, and condensed steam will all be treated in the same manner. The most involved wastewater treatment was chosen due to the excess HMDA and adipic acid that will be in the waste water treatment due to the polymerization reactor not achieving 100% conversion. The capacity of water produced by the process will be treated properly at a nearby water treatment plant in Calvert City, Kentucky. The total cost per year of treating the wastewater is $2,705,000 (*Table 25* below for wastewater). This water will then be disposed in accordance with the Clean Water Act and Pollution Prevention Act.

Table 25: Wastewater Treatment Costs		
Wastewater treatment (Tertiary)	lbm/yr	Cost/yr
Water produced by the process	8.76E+08	$ 22,000
C.W. Return and condensed steam	1.05E+11	$ 2,682,000

Environmental considerations and sustainability had to be considered for this process. The raw materials adipic acid and HMDA are harmful if released to the environment. Special care was taken to control the storage and transportation of these chemicals. For the process, water will be treated and recycled when possible. Steam and cooling water will cycle through the heat exchangers and condensers. If blow down ratio is kept small by controlling process equipment, much of the water can be conserved.

While the scope of this project did not include deriving adipic acid and HMDA from other chemicals, this could be considered to add an element of sustainability to the process. Adipic acid is typically made from cyclohexanone in petroleum processing. However, several studies have shown that adipic acid can be made from biomaterials [38]. Adipic acid for production of Nylon 6 6 has to be of a very high quality and purity in order to produce a polymer that can be processed. This was originally a problem with bio-based adipic acid, but more work is being done to improve the process. This breakthrough could significantly impact the sustainability of Nylon 6 6 production.

Other Important Considerations

Control Strategy Description

The process is controlled using several common controls as listed in *Table 26.* There are two unusual control conventions used. One is on hoppers TK-101 and TK-103. The raw materials used in the production of Nylon 6 6, adipic acid and HMDA, are solids. A mass flow control is used to ensure the correct amount of each chemical is flowing into M-100 and M-101. This can be done by weight, solid level sensors, or controlled by a rotary valve or mass flow screw feeder. The best method will depend on the spatial organization of the plant and the specific flow paths of the hoppers chosen. The other unusual convention is for the pH control of the Nylon salt reactor, R-100. The Nylon salt has to form in a one-to-one ratio for the Nylon polymer to form correctly. It has been studied that at a specific pH, the concentration of adipic acid and HMDA is one-to-one [39]. Measuring the pH is easier, more reliable, and more accurate than trying to control just the concentration of the aqueous mixtures coming into the reactor. Solubility data is available, but the pH is a more reliable control.

Control Variables and manipulated variables are listed in *Table 26*. Heat exchangers and condensers are controlled with a feedback loop where temperature of the process stream out needs to be set and flow rate of steam or cooling water is adjusted to keep the temperature at the set point. Nitrogen blankets in TK-102 and TK-103 are controlled with pressure. This systems ensures that the HMDA is safely stored and will not degrade due to its hygroscopic qualities. Level is controlled to M-100 and M-101 by a flow control valve. Level is controlled in R-100, R-101 and R-102 by control valves that adjust the flow rate out of reactor on the discharge side of the following pump. Pressure has to be controlled in R-101 because water has to be at certain conditions to evaporate and create a salt slurry that will flow to R-102. To reach a certain degree of polymerization, a certain amount of water has to leave the mixture. This requires specific high pressure and temperatures. If the temperature and pressure are too low, the Nylon salt will not polymerize. If the temperature gets too high, the polymer will start to degrade, forming CO2 and creating a build-up of pressure. If too much water is taken out, the reaction moves from being endothermic to exothermic and may overheat the reactor. Thus the temperature and pressure will be tightly regulated at the temperatures and pressures listed in the stream tables.

During start up, the polymerization reactor should be carefully monitored so that it does not exceed its practical stability limit. There is a pressure control, liquid level control and a heater on this reactor in order to ensure that this does not happen. A cooling system on this reactor should also be considered in the case that the reactor does start to overheat, and control is lost on the process. The mechanical processing equipment at the end has temperature controls to ensure that the Nylon is sufficiently dried and cooled for storage and transport.

The process is designed to be continuous, so each process vessel has the potential to affect what is happening in the next stage of the process. This is mitigated by the control strategy in several ways to prevent loss and ensure safe operations. M-100, M-101, and R-100 are sized to withstand extra hold up time. If something occurs in R-101 or R-102, or there is a malfunction in the extruder, no product is lost. If there are changes to the flow rate of deionized water, availability of raw materials or poor mixing in R-100, then R-101 and R-102 have enough controls to adjust the temperature and pressure in accordance with the new lower flowrates.

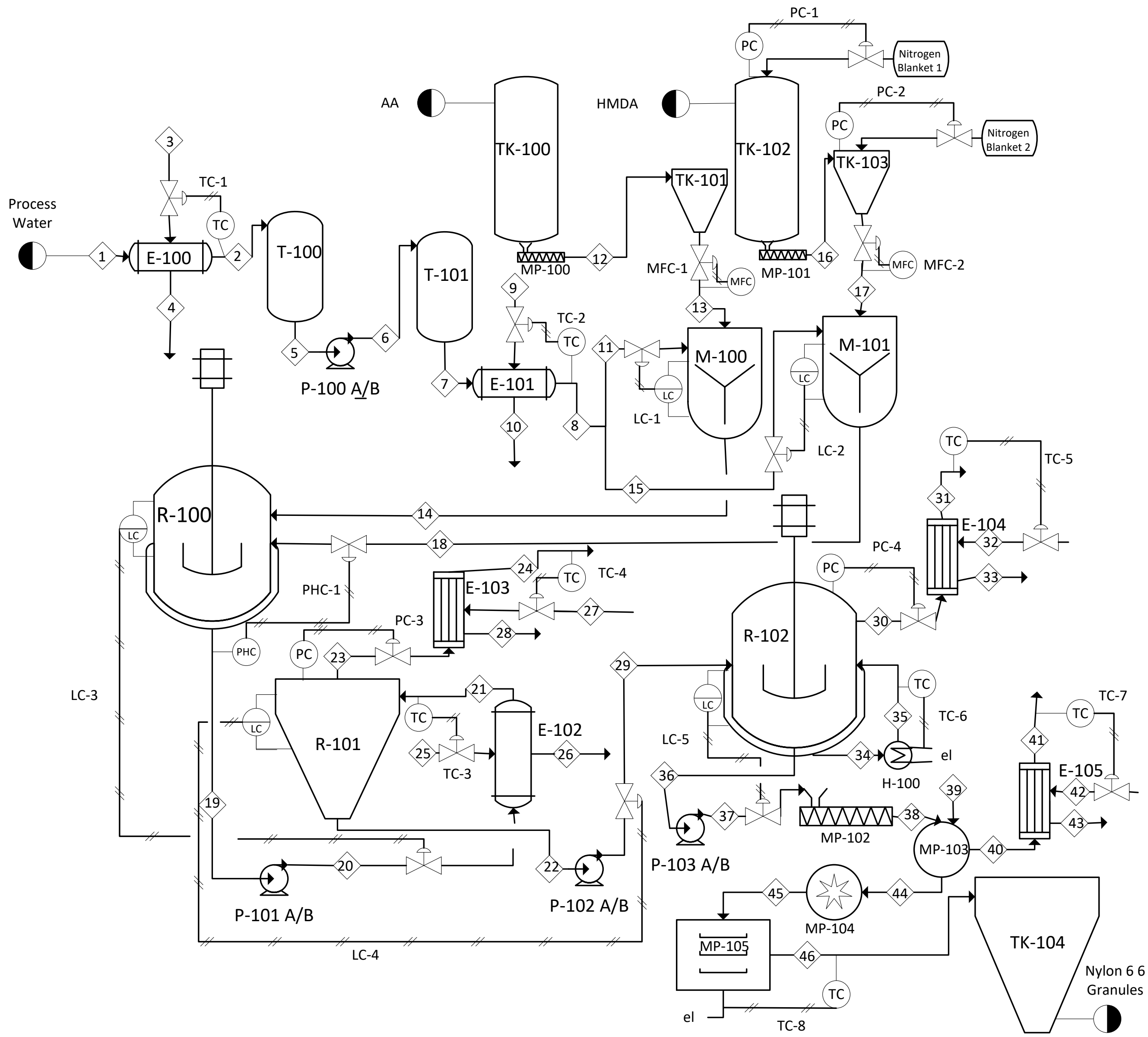

Figure 3: Control Strategy Process Flow Diagram

Table 26: Control Strategy Variables				
Equipment/System Controlled	**Loop**	**PFD ID**	**Control Variable**	**Manipulated Variable**
Nitrogen Blanket	PC-1	Nitrogen Blanket-1	Pressure in TK-102	Flow of Nitrogen
	PC-2	Nitrogen Blanket-2	Pressure in TK-103	Flow of Nitrogen
Heat Exchangers	TC-1	E-100	Temperature of 2	Flow Rate of 3 (Steam)
	TC-2	E-101	Temperature of 8	Flow Rate of 9
	TC-3	E-102	Temperature of 21	Flow Rate of 25
Condensers	TC-4	E-103	Temperature of 24	Flow Rate of 27 (Cooling Water)
	TC-5	E-104	Temperature of 31	Flow Rate of 32
	TC-7	E-105	Temperature of 41	Flow Rate of 42
Heater	TC-6	H-100	Temperature of 35	Electricity/Utility
Dryer	TC-8	MP-105	Temperature of 46	Electricity/Utility
Hoppers/Mixers	MFC-1	TK-101	Flow Rate of 13	Mass Flow through line 13
	MFC-2	TK-103	Flow Rate of 17	Mass Flow through line 17
	LC-1	M-100	Liquid Level in mixer	Flow Rate of 11
	LC-2	M-101	Liquid Level in mixer	Flow Rate of 15
Nylon Salt Formation	pHC-1	R-100	pH in reactor	Flow Rate of 18
	LC-3		Liquid Level in reactor	Flow Rate of 20
Crystallizer/Evaporator	PC-3	R-101	Pressure in reactor	Flow Rate of 24
	LC-4		Liquid Level in reactor	Flow Rate of 29
Polymerization Reactor	PC-4	R-102	Pressure in reactor	Flow Rate of 31
	LC-5		Liquid Level in reactor	Flow Rate of 37

Abbreviations:	LC	Level Control	
	MFC	Mass Flow Control	
	PC	Pressure Control	
	pHC	pH Control	
	TC	Temperature Control	

Startup Including Additional Equipment

The startup for the continuous stirred tank reactor for the polymerization process is semi-batch. The behavior of the temperature of the reaction and how it reaches steady state is important to this process. Polymath was used to create a chemical reaction model to analyze the startup conditions of the CSTR, R-102, that creates the molten Nylon 6 6. The temperature for this start up process was modeled to determine if there would be an overshoot in temperature that would degrade the polymer on its approach to steady state operation. Based on the Polymath simulation, which can be found on Figure A.3 and A.4 in the Appendix section of this report, the temperature of the reaction approaches steady state after five hours.

Location Considerations

The plant will be located in Calvert City, Kentucky. The temperatures are moderate and range around 40 °F in cooler months and around 70 °F in the warmer seasons. Calvert City lies close to tornado alley, so extra safety precautions will be taken to ensure that there is an emergency procedure for visitors and employees if dangerous weather conditions were to occur. The average temperature of groundwater in this region is 52 °F [40], so this was the temperature used for the process water at the plant.

Process optimization

For the process of creating the Nylon salt for the reaction, the solubility of the adipic acid and HMDA in water is an important consideration. Adipic acid is significantly less soluble than HMDA, thus it requires a larger mixer to dissolve the solid in deionized water, as well as increases the size of the Nylon salt formation reactor. Therefore, in order to increase the solubility of the adipic acid in water, the temperature of this water was increased by addition of a heat exchanger, E-101.

Another important decision in optimization was selecting the jacket fluid used for the polymerization reactor, R-102. Temperature is a key parameter in ensuring that the reaction is driven to a high enough temperature that the monomers continue to react. However, if the temperature within the reactor becomes too high, this will cause degradation of the polymer. This is why Dowtherm was selected as the jacket fluid because it provides better heat transfer than high pressure saturated steam at a lower pressure [2].

67% Turndown Case

A turndown case when only 67% of the Nylon 6,6 mass flowrate was available was analyzed to see the effects of operating the plant. The turndown case is beneficial for when the plant experiences a drop in demand. In Table 27, the major parameter used for sizing each piece of equipment was recorded to see the difference in size or capacity when only 67% of the capacity is used. The extruder, casting wheel, and dryer were not affected by the change due to the operating time and power still being required regardless of capacity change. During the turndown case, the equipment will be operating at less optimum conditions throughout the system. The decreased capacity means that all storage tanks will be able to hold more raw material and Nylon granules. There appears to be no significant concerns for operating these pieces of equipment at a lower capacity. Further detailed design will need to be conducted to determine if the pumps will be able to handle a lower capacity. The process will just not be as efficient when it is not operated at full capacity. Utility costs will decrease due to the decrease in pump power and heat exchanger steam or cooling water (*Table 28*). Due to a lower capacity, the amount of Nylon produced is not sufficient to produce an economically attractive net present value for a ten year project life. The net present value was negative $6,299,000 (Table 30). A longer project life may yield a positive net present value, but within ten years, it is not recommended to run the facility consistently at 67% capacity. It would be better to operate at full capacity and store the Nylon granules for later use when demand increases.

Table 27: Equipment Changes Based on Capacity			
PFD Label	Major Parameter of Equipment	100% Capacity Case	67% Capacity Case
E-100	Steam Mass Flowrate (lb/hr)	5943	3950
T-100	Volume (ft^3)	177	131
P-100 A/B	Power (hp)	2.34	1.7
T-101	Volume (ft^3)	177	131
E-101	Steam Mass Flowrate (lb/hr)	2652	1763
TK-100	Days of Storage Available	6	9
MP-100	Drive Power (hp)	1.9	1.6
TK-101	Hold-up Time (hr)	2	3
TK-102	Days of Storage Available	6	9
MP-101	Drive Power (hp)	1.7	1.5
TK-103	Hold-up Time (hr)	2	3
M-100	Residence Time (hour)	0.5	0.75
M-101	Residence Time (hour)	0.5	0.75
R-100	Residence Time (hour)	0.5	0.75
P-101 A/B	Power (hp)	27	19
E-102	Steam Mass Flowrate (lb/hr)	16641	11061
R-101	Water Vapor Flowrate (lb/hr)	103579	68847
E-103	Cooling Water Mass Flowrate (lb/hr)	3.26E+06	2.70E+06
P-102 A/B	Power (hp)	3.0	2.0
R-102	Volume (ft^3)	718	481
E-104	Cooling Water Mass Flowrate (lb/hr)	60325	41004
H-100	Heat Duty (GJ/hr)	0.78	0.46
E-105	Cooling Water Mass Flowrate (lb/hr)	7.51E+04	4.69E+04
P-103 A/B	Power (hp)	24.1	16.2
MP-102	Drive Power	No changes due to operating conditions	
MP-103	Water Vapor Flowrate (lb/hr)	1003	645
MP-104	Drive Power	No changes due to operating conditions	
MP-105	Drive Power	No changes due to operating conditions	
TK-104	Days of Storage Available	4	5.3

Table 28: Utilities Requirement and Yearly Costs for 67% Capacity Case		
Types/Location	**Capacity**	**Cost**
Steam from boilers	lbm/yr	$/year
high pressure / E-102	9.21E+07	$1,251,000
med pressure / E-100 and E-101	4.75E+07	$638,000
Cooling tower water	lbm/yr	
condenser-crystallizer	1.81E+10	$122,000
inside casting wheel	208050	$1
outside casting wheel	5.37E+06	$36
condenser-polymerization CSTR	3.41E+08	$2,300
condenser-casting wheel	3.91E+08	$2,640
Other Water	lbm/yr	
Process water / into Deionize tank	5.78E+08	$554,000
Thermal system	GJ/yr	
Dowtherm boiler / Polymerization CSTR	3.84E+03	$47,000
Electrical	hp.hr/yr	
pump / btw di water tanks	1.41E+04	$631
pump / to the crystallizer	1.61E+05	$7,210
pump / to polymerization CSTR	1.64E+04	$732
pump / to extruder	1.35E+05	$6,022
mixer / aq. HMDA tank	7.66E+03	$342
mixer / aq. adipic acid tank	5.07E+04	$2,266
agitation / aq. Nylon salt cstr	5.84E+04	$2,608
agitation / polymerization cstr	1.35E+05	$6,018
drive / extruder	1.33E+05	$5,950
drive / casting wheel	8.37E+05	$37,000
drive / chopper	8.37E+05	$37,000
drive / dryer	1.00E+06	$45,000
drive / conveyer HMDA	1.25E+04	$558
drive / conveyer Adipic acid	1.33E+04	$595
TOTAL COST		$2,783,525

Table 29: Manufacturing Costs for 67% Capacity Case	
Cost Item	**$/year**
Direct Manufaturing Costs	
Raw Materials	$63,017,000
Waste Treatment	$1,798,000
Utilities	$2,784,000
Operating Labor	$3,676,000
Direct supervisory and clerical labor	$662,000
Maintenance and repairs	$1,311,000
Operating Supplies	$197,000
Laboratory Charges	$551,300
Total Direct Manufacturing Costs	**$73,994,000**
Fixed Manufacturing Costs	
Plant Overhead Costs	$3,389,000
Total Manufacturing Costs	**$3,389,000**
General Manufacturing Expenses	
Administration Costs	$847,000
Distribution and Selling Costs	$5,827,000
Total General Manufacturing Costs	**$6,674,000**
Total Costs	**$84,057,000**

Table 30: 67% Capacity Cash Flow Diagram

Project Title:	Manufacturing Facility for Nylon 6 6, Turndown case of 67% capacity
Corporate Financial Situation:	Expense
Minimum Rate of Return, i*:	0.15
	1 =
Other relevant project info.:	$1,000
MACRS Depreciation Scale at 5 years:	0.2000 0.3200 0.1920 0.1152 0.1152 0.0576

End of Year	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027
	0	1	2	3	4	5	6	7	8	9	10
Production, "MM lb/year"		57	57	57	57	57	57	57	57	57	57
x Sales Price, $/lbm Nylon 6,6	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53
Sales Revenue = Net Revenue ($/yr)	-	87,134	87,134	87,134	87,134	87,134	87,134	87,134	87,134	87,134	87,134
-Manufacturing Cost		(84,057)	(84,057)	(84,057)	(84,057)	(84,057)	(84,057)	(84,057)	(84,057)	(84,057)	(84,057)
-Depreciation		(4,370)	(6,991)	(4,195)	(2,517)	(2,517)	(1,258)	0	0	0	0
-Writeoff											
-Working Capital											(3,277)
Taxable Income	0	(1,293)	(3,915)	(1,119)	559	559	1,818	3,076	3,076	3,076	(201)
-Tax @ 40%	0	517	1,566	447	(224)	(224)	(727)	(1,230)	(1,230)	(1,230)	80
Net Income	0	(776)	(2,349)	(671)	336	336	1,091	1,846	1,846	1,846	(121)
+Depreciation	-	4,370	6,991	4,195	2,517	2,517	1,258	-	-	-	-
+Writeoff	-	-	-	-	-	-	-	-	-	-	-
+Working Capital	-	-	-	-	-	-	-	-	-	-	3,277
-Grassroots Cost (FCI)	(21,848)										
Cash Flow	(21,848)	3,593	4,642	3,524	2,852	2,852	2,349	1,846	1,846	1,846	3,156
Discount Factor (P/F)	1.0000	0.8696	0.7561	0.6575	0.5718	0.4972	0.4323	0.3759	0.3269	0.2843	0.2472
Discounted Cash Flow	(21,848)	3,125	3,510	2,317	1,631	1,418	1,016	694	603	525	780
NPV @ i*=	(6,229)	*Economically not attractive since NPV < 0*									
DCFROR =	5.91%	*Economically not Attractive since DCFROR < i**									

Manufacturing Costs (Exclusive of Capital Requirements)

The analysis and evaluation of manufacturing costs for this project were conducted based on the manufacturing cost correlations available in the textbook *Analysis, Synthesis, and Design of Chemical Processes* [2]. Manufacturing costs are categorized into: direct manufacturing costs, fixed costs, and general expenses. Direct manufacturing costs for this process are outlined in *Table 31.* The raw materials costs were based on the provided quote from INVISTA for adipic acid and HMDA.

Table 31: Raw Material Costs	
Raw Material Information	**Value**
HMDA supply rate, metric tonne/year	2.16E+04
Adipic acid supply rate, metric tonne/year	2.72E+04
HMDA purchase price, $/metric tonne	$2,500
Adipic acid purchase price, $/metric tonne	$1,500
Total Raw Material Cost, $/year	**$94,808,000**

Operating labor costs account for employment costs required for plant operation. The number of operators was estimated based on the major equipment used in the process (excluding pumps and storage vessels). The most current hourly labor cost for May 2015 is shown in *Table 32* [41]. Through a scale up procedure of employment cost indexes, the June employment cost index was calculated. The data for the employment cost index was retrieved from the *Bureau of Labor Statistics-Employment Cost Index for Wages and Salaries* as well [41]. The employment cost index used in this project was from June 2016. Depending on when the start-up of the project will be implemented, an escalation in the employment cost index would need to be accounted for.

Table 32: Operating Labor Costs	
Operating Labor Information	**Value**
Employment Cost Index (June, 2016)	127.1
Employment Cost Index (Dec 2015)	123.8
Operating labor ($/year)	$256,000
Operating hours/year	8322
Hourly labor cost ($/hr) (May 2015)	$30.73
Operators	14
Number of Operators per Shift	3.08
Number of Major Process Equipment	14
Number of Processing Steps, P	0
Total Raw Material Cost, $/year	**$94,808,000**

The cost analysis for waste water treatment is accounted for by using tertiary wastewater treatment. Other types of direct manufacturing costs that must be accounted for include: direct supervisory and clerical labor, maintenance and repairs, operating supplies and laboratory charges. These additional costs are estimated using correlations between the direct manufacturing costs, fixed costs, and general expenses. In addition, the costs related to patents and royalties were not considered in this evaluation since this process is well known and patents have expired.

The fixed manufacturing costs and the general manufacturing expenses were evaluated also utilizing the midpoint values of the correlation factors [2].

In fixed manufacturing costs, the cost regarding depreciation, local taxes, and insurance were not evaluated utilizing the midpoint value of multiplication factor. The local taxes rate was accounted in the effective tax rate that was used in the ten-year-project life cash flow diagram which approximately is 40% regarding the U.S. federal corporate tax rate and additional state corporate taxes [42]. The method of modified accelerated cost recovery system (MACRS) depreciation with a 5-year class life property was applied to implement the account for depreciation in the cash flow diagram. Due to this facility being an industrial environment, no research and development costs will be included in the general manufacturing expenses.

Table 33: Manufacturing Cost for 100% Capacity Case	
Cost Item	**$/year**
Direct Manufaturing Costs	
Raw Materials	**$94,808,000**
Waste Treatment	**$2,705,000**
Utilities	**$4,132,000**
Operating Labor	**$3,676,000**
Direct supervisory and clerical labor	$662,000
Maintenance and repairs	$1,311,000
Operating Supplies	$197,000
Laboratory Charges	$551,000
Total Direct Manufacturing Costs	**$108,040,000**
Fixed Manufacturing Costs	
Plant Overhead Costs	$3,389,000
Total Manufacturing Costs	**$3,389,000**
General Manufacturing Expenses	
Administration Costs	$847,000
Distribution and Selling Costs	$8,340,000
Total General Manufacturing Costs	**$9,186,609**
Total Costs	**$120,615,897**

Economic Analysis
To evaluate the profitability of the project, the NPV, DCFROR and payback period were calculated on an expense basis. It was assumed that financial situation would be considered as an expense, because although the facility is grassroots, it was designed at the specification of a company. This new facility would be considered a branch of the parent company.

Depreciation was calculated using the Modified Accelerated Cost Recovery System (MACRS) using 5 year depreciation. This was chosen based on the criteria set out by the IRS [43] [44]. Research led to the assumption of a hurdle rate of 15 %. This rate can change based on increased investment risks, such as changes in the market, or new competitors [45]. Taxes were estimated at 40%. The washout assumption was used to estimate a constant profit margin. The net revenue is based on selling Nylon at $ 1.53 / lbm which was based off of a report from Independent Chemical Information Services [46]. The actual costs and will vary with economic trends, escalation and inflation, but sales costs can be changed to adjust for that.

The net present value of the process is $ 12,916,000 with a DCFROR of 30.4%. The discounted payback period was then calculated to be 4.11 years. This means that after just over 4 years, the facility will have paid off the initial investment and will be making money based on the discounted cash flow. *Table 37* is the cash flow diagram used for the project. The economics suggest that it is beneficial to continue with the design of the facility for Nylon 6 6 granules.

Sensitivity
A single variable sensitivity analysis was performed on the DCFROR for manufacturing costs, annual profit, and fixed capital investment. These variables were estimated to be the most vulnerable to changes. The results are summarized in *Table 35* and the tornado chart in Figure 4. The change in each variable was estimated separately. A large amount of the manufacturing cost was the raw material cost, so raw material costs were looked at to find a reasonable amount of change in Manufacturing costs. Adjusting prices of raw materials by about ten cents per pound created a 10 % change in manufacturing costs. Ten cents was assumed to be a reasonable change due to the order of magnitude of the prices given by Invista, in addition to price trends found for raw materials [46]. Fixed capital investment was estimated with the grassroots equation [2]. The range given for the grassroots estimate was large enough to make 25% a reasonable variation. This value was used to adjust the grassroots change. The change in annual profit was based off of predictions and fluctuations found in price reports for Nylon 6 6 [46]. This translated to a change of 3%.

By analyzing the tornado chart for the three variables, it can be seen that manufacturing costs have the greatest effect on the DCFROR. Annual profit and capital investment have comparable best and worst DCFROR values. For the multivariable sensitivity analysis, the best and worst case scenarios were evaluated for all three variables at once (*Table 34*). The best case scenario is with manufacturing costs and fixed capital investment minimized, and annual profits maximized. This created a DCFROR of 97%. The worst case scenario with increased manufacturing costs and fixed capital investment and lowered annual profit does not produce an investment that makes money.

The breakeven costs were found for adipic acid, HMDA, and Nylon 6 6, and are summarized in *Table 36*. This means that there is a margin where the process is still profitable if the price of Nylon granules drops below the predicted value. This is mitigated by only a small rise in the price of HMDA and adipic acid.

Table 34: Multivariable Sensitivity Analysis			
	Best	Expected	Worst
Variable	$ 108,399,000	$ 120,616,000	$ 130,898,000
Manufacturing Costs	$ 134,000	$ 130,000	$ 126,000
Annual Profit	$ 16,386,000	$ 21,848,000	$ 27,310,000
Fixed Capital Investment	97.11%	30.43%	0%

Table 35: Single Variable Sensitivity Analysis			
	Rate of Return, %		
Variable	**Best Case**	**Worst Case**	**Range**
Manufacturing Costs	67.2%	-33.2%	100.5%
Annual Profit	42.8%	16.5%	26.3%
Fixed Capital Investment	43.3%	22.0%	21.2%
Base Case DCFROR is 30.4%			

Table 36: Breakeven Values for Process Components	
Component	Unit, $/lb
Nylon	1.48
HMDA	1.22
Adipic Acid	0.75

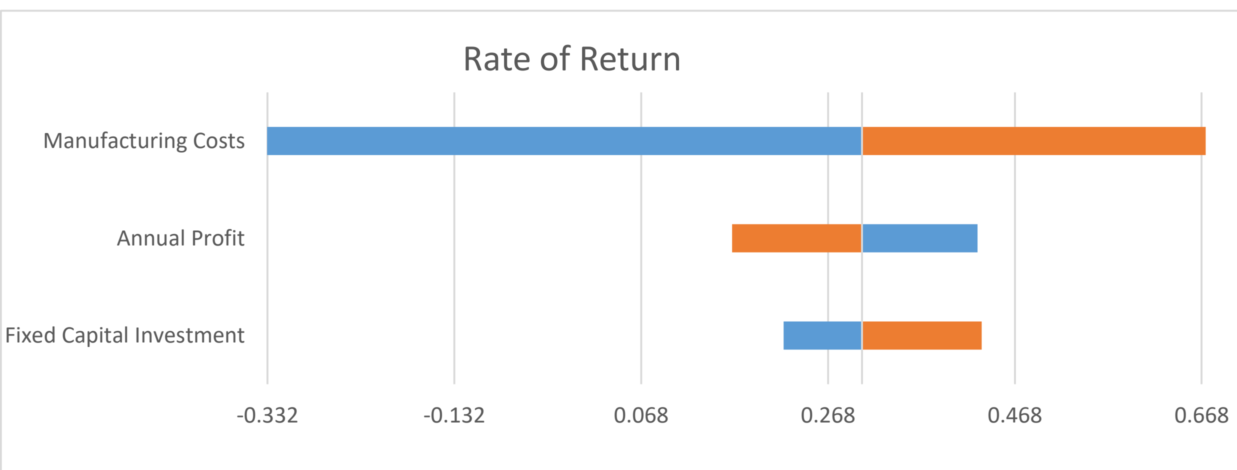

Figure 4: Tornado Chart for Single Variable Sensitivity Analysis

Table 37: 100% Capacity Case Cash Flow Diagram

Project Title:	Manufacturing Facility for Nylon 6 6						
Corporate Financial Situation:	Expense						
Minimum Rate of Return, i*:	0.15						
	1 =						
Other relevant project info.:	$1,000						
MACRS Depreciation Scale at 5 years:		0.2000	0.3200	0.1920	0.1152	0.1152	0.0576

End of Year	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027
	0	1	2	3	4	5	6	7	8	9	10
Production, "MM lb/year"		85	85	85	85	85	85	85	85	85	85
x Sales Price, $/lbm Nylon 6,6	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53
Sales Revenue = Net Revenue ($/yr)	-	130,050	130,050	130,050	130,050	130,050	130,050	130,050	130,050	130,050	130,050
-Manufacturing Cost		(120,616)	(120,616)	(120,616)	(120,616)	(120,616)	(120,616)	(120,616)	(120,616)	(120,616)	(120,616)
-Depreciation		(4,370)	(6,991)	(4,195)	(2,517)	(2,517)	(1,258)	0	0	0	0
-Writeoff											
-Working Capital											(3,277)
Taxable Income	0	5,065	2,443	5,239	6,917	6,917	8,176	9,434	9,434	9,434	6,157
-Tax @ 40%	0	(2,026)	(977)	(2,096)	(2,767)	(2,767)	(3,270)	(3,774)	(3,774)	(3,774)	(2,463)
Net Income	0	3,039	1,466	3,144	4,150	4,150	4,905	5,660	5,660	5,660	3,694
+Depreciation	-	4,370	6,991	4,195	2,517	2,517	1,258	-	-	-	-
+Writeoff	-	-	-	-	-	-	-	-	-	-	-
+Working Capital	-	-	-	-	-	-	-	-	-	-	3,277
-Grassroots Cost (FCI)	(21,848)										
Cash Flow	(21,848)	7,408	8,457	7,338	6,667	6,667	6,164	5,660	5,660	5,660	6,971
Discount Factor (P/F)	1.0000	0.8696	0.7561	0.6575	0.5718	0.4972	0.4323	0.3759	0.3269	0.2843	0.2472
Discounted Cash Flow	(21,848)	6,442	6,395	4,825	3,812	3,315	2,665	2,128	1,850	1,609	1,723
NPV @ i*=	12,916	*Economically attractive since NPV > 0*									
DCFROR =	30.4%	*Economically Attractive since DCFROR > i**									
Undiscounted Payback Period (yrs)	2.82										
Discounted Payback Period (yrs)	4.11										

Conclusions

The Nylon 6 6 granule production process yielded a net present value of $12,916,000 and a DCFROR of 30.4%. Since the net present value is positive, and the DCFROR is greater than the hurdle rate, this is an economically attractive investment. The discounted payback period for this process will be 4.11 years when estimated with a ten year project life. This process produces 85 MM pounds per year of Nylon 6 6 granules through a continuous extrusion process. The production of this polymer requires a deionization water system to purify Calvert City process water. A bulk storage system will be implemented to contain the adipic acid and HMDA, which will then be mixed to form aqueous solutions. The mixture reacts to form Nylon salt which will then be processed by an evaporative crystallizer system. A polymerization reactor is crucial to the process to achieve the desired conversion and produce molten Nylon. The mechanical processing equipment extrudes the molten Nylon and is then cast, chopped, and dried to be prepared for customers. The Nylon 6 6 produced in this process is sold as granules. The Nylon 6 6 is kept as granules so that the company's customers may melt the granules again and be form them into fibers with varying lengths and diameters, depending on the use. The Nylon granules produced will be colorless, so dying can be implemented when further processing occurs.

Recommendations

It is recommended that this Nylon 6 6 granule facility be implemented due to the economically attractive net present value and DCFROR. The granules provide more versatility to potential customers needs when color, length, and diameter are a concern. In order to decrease raw material costs, it is recommended that the Nylon plant include an HMDA and adipic acid manufacturing addition. By producing these components on site, the required input could be better controlled and the materials would be significantly cheaper. Even though this requires additional equipment, it will still lead to a profitable outcome by eliminating the extra expense of delivery and going through different vendors. The current plant designed will be in a location that will allow for adequate space in the design layout to accommodate this future design. Further research and development regarding space time in the polymerization reactor should be implemented in order to optimize the polymerization reactor. Additional hazard analyses should be conducted in order to ensure that the reactors and other high pressure and temperature systems will not result in any dangerous conditions. It is recommended that all employees and visitors be involved in the safety process to ensure that everyone is aware of the potential dangers in this plant.

Acknowledgements

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AIChE Design Project Appendix

Group #_____

March 9, 2017

List of Tables

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Equipment Sizing and Costing Spreadsheet Attachments:

Table A.1: Heat Exchanger E-100 Sizing and Costing

Heated process water			
E-100: Heat Exchanger (Fixed tube) (shell: steam and tube: Process water)			
Sizing:	ft^2	m^2	
Area	336.909	31.300	
Uo (Btu/hr*ft^2*°F)	50	(Heuristic from Turton for liquid to liquid)	
Temperatures	℃	°F	
Tcool,in	11.11	52	
Tcool,out	38	100.4	
Temperature approach	153.67	308.6	
Thot,in	191.67	377	(med. steam)
Thot,out	191.67	377	
Log Mean Temperature	148.97	300.15	
Correction Factor, F	1		
P	0.15		
R	0.00		
P'	0.15		
Heat Duty (Btu/hr)	5.06E+06		
Latent Heat (Btu/lbm)	850.73	high pressure steam	
Steam mhot (lbm/hr)	5943.31	Utility cost	
Process water mcold (lbm/hr)	104466.00	(Jessica and Laurent)	
Heat Capacity of Water(Btu/lbm*°F)	1	Engineering toolbox	
Purchased Equipment Costs			
Result	C^o_p	$ 17,331	
Variables/Info	Equipment Type	HEX	
	Equipment Description	fixed tube	
(*unit)	Area, m2	**32.0**	(in the range)
(to check)	min	10	
	max	1000	
	K1	4.3247	
	K2	-0.303	
	K3	0.1634	
Pressure Factors			
Result	Fp	1.02	
	Fp, process vessels		
Variables/Info	Equipment Type	HEX	
	Equipment Description	shell and tube	
psia	P med. at. Steam	189.70	
psia	P process water in	105.00	
psia	Design pressure, P	155.00	
(*barg)	Design pressure, P	9.67	(in the range)
(to check)	min	5	
	max	140	
	C1	0.03881	
	C2	-0.11272	
	C3	0.08183	
	Diameter, D		
Bare Module Cost			
Result	C_{BM}	$ 57,499.39	
	$C_{BM, process\ vessel}$		
	Equipment Type	HEX	
	Equipment Description	shell and tube	
	MOC	CS	
	Identificaiton number	1	
	F_M	1	
	B1	1.63	
	B2	1.66	
Purchased Cost, Cp		$ 24,193.93	
Installed Cost, C_{BM}		**$ 78,949**	
Year 2001	C.I.	397	
Desired year (2016)	C.I.	545.1	

Table A.2: Deionized Water System T-100 and T-101 Sizing and Costing

Mixed Bed Deionizer	2 in series	
Temperature (°F)	100.4	5-7 psi pressure drop
Sizing		
Capacity (gpm)	211.4	to 220
Diameter (ft)	5	
Height (ft)	9	
Volume (ft^3)	122.71	
Volume (gal)	917.99	
% Anion Resin	60	Chloride resin
% Cation Resin	40	Hydrogen resin
Resin Volume (ft^3)	54	
Total Volume (ft^3)	176.71	
Costing	Vertical Process Vessel	
K1	3.4974	
K2	0.4485	
K3	0.1074	
Volume (m^3)	5.00	
logCp0	3.86	
Cp0	$7,304	
P (psig)	85.3	
P (barg)	5.9	
D (ft)	5.000	
D (m)	1.52	
Fp	1.5	
Purchase Cost:		
Identification Number	18	Carbon Steel
Fm	1	
Cp (2001)	$10,839	
Cp (2017)	$14,882	
Installed Cost:		
Fm	1	
B1	2.25	Table A.4
B2	1.82	
Cbm (2001)	$36,161	
Cbm (2017)	$49,650	One Deionizer
Total Cbm for both Mixed Bed Deionizers	**$99,301**	
Installation Cost	$34,768	

Table A.3: Pump P-100 Sizing and Costing

Pump between DI water tanks			
P-100: Pump Sizing with an elvation change			
Sizing			
Inlet Flow Rate of DI water (lbm/hr)	104466.00	Obtained from Heated DI water HEX	
DI water density (lbm/ft3)	61.99	Engineering toolbox	
Inlet Flow Rate of DI water (gpm)	210.10	unit conversion	
Inlet pressure of DI stream (psia)	95	Laurent and Jessica	
DI Water Tank 2 pressure (psia)	100		
Height of di water tank 2 (ft)	9.00	Laurent and Jessica	
ΔP hydrostatic (psi)	3.90	Laurent and Jessica	
ΔP Necessary (psia)	8.90	$\Delta P_{pump}+\Delta P_{hydrostatic}+\Delta P_{losses}$	
ε_{pump}	0.52	Interpolated From Turton Table 11.9	
W_{pump} (hp)	2.10	Flow Rate*$\Delta P/\varepsilon_{pump}$	
ε_{driver}	0.9	Estimation from Turton 11.5, midpoint	
$W_{purchased}$ (hp)	2.34	$W_{pump}/\varepsilon_{driver}$	
$W_{purchased}$ (kW)	1.74	Unit conversion	
Costs:			
Purchased Equipment Costs			
Result	C^o_p	$	2,576.71
Variables/Info	Equipment Type	Pump	
	Equipment Description	Centrifugal	
(*unit)	Capacity: Shaft power (kW)		**1.74**
(to check)	min		1
	max		300
	K1		3.3892
	K2		0.0536
	K3		0.1538
Pressure Factors			
Result	Fp		0.98
Variables/Info	Equipment Type	Pump	
	Equipment Description	Centrifugal	
psia	Operating pressure		103.90
psia	Design pressure, P		153.90
(*barg)	Design pressure, P		9.60
(to check)	min		10
	max		100
	C1		-0.3935
	C2		0.3957
	C3		-0.00226
(*unit)	Diameter, D (m)		
Bare Module Cost			
Result	C_{BM}	$	14,111.06
	Equipment Type	Pump	
	Equipment Description	Centrifugal	
	MOC	SS	
	Identificaiton number		39
	F_M		2.7
	B1		1.89
	B2		1.35
Purchased Cost, C_p		$	9,398.84
Installed Cost, C_{BM}		**$**	**19,375**
Installation Cost		$	9,976.31
Year 2001	C.I.		397
Desired year (2016)	C.I.		545.1
Total cost including spare pump	**$ 38,750**		

Table A.4: Heat Exchanger E-101 Sizing and Costing

Heated DI Water			
E-101: Heat Exchanger (Fixed tube) (shell: steam and tube: DI water)			
Sizing:	ft^2	m^2	
Area	169.880	15.782	
Uo (Btu/hr*ft^2*°F)	50	(Heuristic from Turton for liquid to liquid)	
Temperatures	℃	°F	
Tcool,in	38.00	100.4	
Tcool,out	50	122	
Temperature approach	141.67	287	
Thot,in	191.67	377	(low p. steam)
Thot,out	191.67	377	
Log Mean Temperature	129.81	265.65	
Correction Factor, F	1		
P	0.08		
R	0.00		
P'	0.08		
Heat Duty (Btu/hr)	2.26E+06		
Latent Heat (Btu/lbm)	850.73	low pressure steam	
Steam mhot (lbm/hr)	2652.38	Utility cost	
Process water mcold (lbm/hr)	104466.00	(Jessica and Laurent)	
Heat Capacity of Water(Btu/lbm*°F)	1	Engineering toolbox	
Purchased Equipment Costs			
Result	C^o_p	$ 15,731	
Variables/Info	Equipment Type	HEX	
	Equipment Description	fixed tube	
(*unit)	Area, m2	**16.0**	(in the range)
(to check)	min	10	
	max	1000	
	K1	4.3247	
	K2	-0.303	
	K3	0.1634	
Pressure Factors			
Result	Fp	1.01	
	Fp, process vessels		
Variables/Info	Equipment Type	HEX	
	Equipment Description	shell and tube	
	P med. P sat steam	189.70	
psia	P stream in	95.00	
psia	Design pressure, P	145.00	
(*barg)	Design pressure, P	8.98	
(to check)	min	5	
	max	140	
	C1	0.03881	
	C2	-0.11272	
	C3	0.08183	
	Diameter, D		
Bare Module Cost			
Result	C_{BM}	$ 52,102.78	
	$C_{BM, process vessel}$		
	Equipment Type	HEX	
	Equipment Description	shell and tube	
	MOC	CS	
	Identificaiton number	1	
	F_M	1	
	B1	1.63	
	B2	1.66	
Purchased Cost, Cp		$ 21,886.60	
Installed Cost, C_{BM}		**$ 71,540**	
Year 2001	C.I.	397	
Desired year (2016)	C.I.	545.1	

Table A.5.: Adipic Acid Bulk Storage TK-100 Sizing and Costing

ADIPIC ACID - Bulk Storage	**Screw Conveyer:**	
	Solids flow Rate (lb/hr)	7,200
*Source is encyclopedia 11	Density (g/cm^3)	1.366
	Volumetric Flow Rate (ft^3/hr)	84.43
Can justify this by saying due to weather conditions etc. need to be able to operate continuously for a 6 days. Can let volume go done to 2 days worth and have a shipment every 4 days.	**For 6 Days Worth of Material:**	
	Mass (lb)	1,036,795.68
	Volume (ft^3)	12,158
*Max heuristic for vertical is 520 m^3	Volume (m^3)	344.3
*Beyond 10,000 gallon means vertical tank on concrete pads	Volume (gallons)	90,948
	Vertical Process Vessel (BULK Solid Adipic Acid Storage)	
*V= pi*D^3 if L/D equals 4	Volume Needed for 6 Days (ft^3)	12,158
*Found based on cylinder and L/D equal to 4. Rounded up to nearest ft.	D (ft)	16.0
***Must manually use solver to get this**	L (ft)	60.5
*This is slightly different from volume needed based on rounding	Actual Volume (ft^3)	12,164
	Actual L/D	3.78
*This is in between 0.1 to 520 range in correlations	**Actual Volume (m^3)**	**344**
	Area of Base (in^2)	28,953
*Should validate that this is safe	PSI on Base (lb/in^2)	35.81
	K1	3.4974
	K2	0.4485
	K3	0.1074
	logCp0	5.327
	Cp0	$ 212,156
	P design (barg) (Atm +50psi)	3.45
	D (m)	4.88
	Fp	2.53
	Installed Cost:	
	Fm	1
	B1	1.49
	B2	1.52
	FBM	5.339
	Cbm (2001)	$ 1,132,778
	Cbm (2016, using CEPCI of 545.1)	$ 1,545,086

Table A.6.: HMDA Bulk Storage TK-102 Sizing and Costing

HMDA - BULK STORAGE	**Screw Conveyer:**	
	Solids flow Rate (lb/hr)	5,726
*SDS, relative density at 77F	Density (g/cm^3)	0.89
	Volumetric Flow Rate (ft^3/hr)	103.07
	For 6 Days Worth of Material:	
	Mass (lb)	824,610.24
	Volume (ft^3)	14,842
*Max heuristic for vertical is 520 m^3	Volume (m^3)	420.3
*Beyond 10,000 gallon means vertical tank on concrete pads	Volume (gallons)	111,023
	Vertical Process Vessel (BULK Solid Adipic Acid Storage)	
*V= pi*D^3 if L/D equals 4	Volume Needed for 6 Days (ft^3)	14,842
*Found based on cylinder and L/D equal to 4. Rounded up to nearest ft.	D (ft)	17.0
***Must manually use solver to get this**	L (ft)	65.5
*This is slightly different from volume needed based on rounding	Actual Volume (ft^3)	14,867
	Actual L/D	3.85
*This is in between 0.1 to 520 range in correlations	**Actual Volume (m^3)**	**421**
	Area of Base (in^2)	32,685
*Should validate that this is safe	PSI on Base (lb/in^2)	25.23
	K1	3.4974
	K2	0.4485
	K3	0.1074
	logCp0	5.414
	Cp0	$ 259,446
	P design (barg) (Atm +50psi)	3.45
	D (m)	5.18
	Fp	2.66
	Installed Cost:	
	Fm	1
	B1	1.49
	B2	1.52
	FBM	5.532
	Cbm (2001)	$ 1,435,370
*This price now includes the phenolic resin lining	Cbm (2016, using CEPCI of 545.1)	$ 1,961,037
	Surface Area Inside tank (m^2)	367
	Thickness of Phenolic Resign Desired (m)	0.00045
	Volume of Phenolic Resin (m^3)	0.17
	Density of Phenolic Resin (g/cm^3)	1.30
	Mass of Phenolic Resin Needed (g)	214,796
	Price of Resin ($/X)	15
	Price to Coat ($)	$ 3,222

Table A.7 and A.8: MP-100 and MP-101 Sizing and Costing

Screw Conveyor	Adipic Acid
Sizing:	
Density (g/cm3)	1.36
Density(lb/ft3)	84.86
Capacity (ft3/hr)	56.78
Height(ft)	16
Length of conveyor (ft)	61.82
Volume (ft3)	12.14
Area(ft2)	97.10
Costing:	
K1	3.61
K2	0.27
K3	0.20
Area (m2)	9.02
Cpo	10991.49
Fbm	1.10
Cbm(2001)	12090.64
Cbm(2016 545.1)	$ 16,601.03

HMD	
Sizing:	
Density (kg/m3)	840.00
Density(lb/ft3)	52.42
Capacity (ft3/hr)	103.46
Height(ft)	16.00
Length of conveyor (ft)	61.82
Volume (ft3)	12.14
Area(ft2)	97.10
Costing:	
K1	3.61
K2	0.27
K3	0.20
Area (m2)	9.02
Cpo	10991.49
Fbm	1.10
Cbm(2001)	12090.64
Cbm(2016 545.1)	$ 16,601.03

Drive:	AA
Length	32.00
RPM	12.08
Fd	18.00
Fb	2.00
Fm	0.50
Ff	1.00
Fp	1.00
efficiency	0.88
Hpfriction	0.03
HpMaterial	0.15
Fo(from table)	3.00
HP	1.60
KW	1.19

Drive:	HMD
Length	32.00
RPM	22.01
Fd	18.00
Fb	2.00
Fm	0.50
Ff	1.00
Fp	1.00
efficiency	0.88
Hpfriction	0.05
HpMaterial	0.17
Fo(from table)	3.00
HP	1.74
KW	1.30

Cost	AA
K1	1.96
K2	1.71
K3	-0.23
Cpo	121.86
FBM	1.50
Fp	1.00
CBM	182.79
CBM (2016)	$ 250.97

Cost	HMDA
K1	1.96
K2	1.71
K3	-0.23
Cpo	140.07
FBM	1.50
Fp	1.00
CBM	210.10
CBM (2016)	$ 288.48

Table A.9.: Adipic Acid Hopper TK-101 Sizing and Costing

ADIPIC ACID - HOPPER	Add Uniform mass flow belt to hopper		
	Adipic Acid Hopper		
	Vertical Process Vessel (Solid Adipic Acid Storage)		
***Desired Hold-Up Time based on Jessica's "Storage and Transport of Solids" Source . This is for half-full. We choose middle of range to be conservative (1 to 3 hours)**	Hold-Up Time (hr)	2	
	Volume (ft^3)	337.7	
*Found based on cylinder and L/D equal to 4. Rounded up to nearest ft.	D (ft)	5.0	
***Must manually use solver to get this**	L (ft)	17.5	*saying L/D equal to 4, I believe this is given suggestion on econ book from library (1 to 4)
*This is slightly different from volume needed based on rounding	Actual Volume (ft^3)	344	*Height and Diameter would differ if doing conical hopper shape instead of cylinder
	Actual L/D	3.50	
*This is in between 0.1 to 520 range in correlations	**Actual Volume (m^3)**	**9.73**	
	K1	3.4974	
	K2	0.4485	
	K3	0.1074	
	logCp0	4.045	
	Cp0	$ 11,103	
	P design (barg) (Atm +50psi)	3.45	
	D (m)	1.52	
	Fp	1.135	
	Installed Cost:		
	Fm	1	
	B1	1.49	
	B2	1.52	
	FBM	3.215	
	Cbm (2001)	$ 35,701	
	Cbm (2016, using CEPCI of 545.1)	$ 48,695	

Table A.10.: HMDA Hopper TK-103 Sizing and Costing

HMDA - HOPPER	Add Uniform mass flow belt to hopper		
	HMDA Hopper		
	Vertical Process Vessel (HMDA Storage)		
***Desired Hold-Up Time based on "Storage and Transport of Solids" Source . This is for half-full. We choose middle of range to be conservative (1 to 3 hours)**	Hold-Up Time (hr)	2	
	Volume (ft^3)	412.3	
*Found based on cylinder and L/D equal to 4. Should round to nearest .5 ft?	D (ft)	6.0	
***Must manually use solver to get this**	L (ft)	15	*saying L/D equal to 4, I believe this is given suggestion on econ book from library (1 to 4)
*This is slightly different from volume needed based on rounding	Actual Volume (ft^3)	424	*Height and Diameter would differ if doing conical hopper shape instead of cylinder
	Actual L/D	2.50	
*This is in between 0.1 to 520 range in correlations	**Actual Volume (m^3)**	**12.01**	
	K1	3.4974	
	K2	0.4485	
	K3	0.1074	
	logCp0	4.107	
	Cp0	$ 12,786	
	P design (barg) (Atm +50psi)	3.45	
	D (m)	1.83	
	Fp	1.262	
	Installed Cost:		
	Fm	1	
	B1	1.49	
	B2	1.52	
	FBM	3.409	
	Cbm (2001)	$ 43,582	
*This price now includes the phenolic resin lining	Cbm (2016, using CEPCI of 545.1)	$ 59,721	
	Surface Area Inside tank (m^2)	32	
	Thickness of Phenolic Resign Desired (m)	0.00045	
	Volume of Phenolic Resin (m^3)	0.0142	
	Density of Phenolic Resin	1.30	
	Mass of Phenolic Resin Needed (g)	18,440	
	Price of Resin ($/kg)	15	
	Price to Coat ($)	276.61	

Table A.11.: Adipic Acid Mixer M-100 Sizing and Costing

ADIPIC ACID - Dissolved Solution		
Mixer: Preparing Adipic Acid in Solution		
Density (g/cm^3)	1.366	*Source: Encyclopedia 11
pH	2.7	
Max Solubility at 50°C or 122°F (g/L)	82.7	*Source: Solubility use table 2: This is the low end of experimental data to be conservative
Solubility Allowing in Calculations (g/L)	74.43	*Chose this 90% of maximum solubility. This was an estimate to make sure completely soluble.
MW of Adipic Acid (g/mol)	146.14	
Desired Residence Time (hr)	**0.5**	*30 minutes based on "Mixer Settler Time" Source
Known Flow Rate of Solid Out (lb/hr)	7,200	
Flow Rate of solid (g/hr)	3,265,849	
Flow Rate of Water Needed (L/hr)	43,878	
Volume of Water in Reactor (L)	21,939	
Volume of Mixer (including solids) (ft^3)	1,634	*Saying here that liquid level is half of the height of the reactor.This will give a hold-up time equal to the residence time.
D (ft)	10.5	
L (ft)	19	
Actual Volume (ft^3)	1,645	
Actual L/D	1.81	
Actual Volume (m^3)	**46.59**	*0.04 to 60 m^3
Reactor-Mixer/Settler for Adipic Acid (Design Textbook)		
K1	4.7116	
K2	0.4479	
K3	0.0004	
Volume (m^3)	46.59	0.04 to 60 m^3
logCp0	5.460	
Cp0	$ 288,361	
FBM (Reactor-Mixer Settler) - Table 4.7	4.0	
Cbm (2001)	$ 1,153,446	
Cbm (2016, using CEPCI of 545.1)	$ 1,573,277	
Utility Cost: Horsepower		
Volume of Fluid (1/2 of Volume calculated based on fluid) (f	817	
Volume of Fluid (gallons)	6,111	
HP	9.167	

Table A.12.: HMDA Mixer M-101 Sizing and Costing

HMDA - DISSOLVED SOLUTION		
Mixer: Preparing HMDA in Solution		
Density (g/cm^3)	0.89	*SDS
pH	12.4	
Solubility Allowing in Calculations (g/L)	637	*This is the only known solubility data and is at 20C so we will say has to be more soluble at 50C so it is safe to assume that this amount will fully dissolve.
MW of HMDA (g/mol)	116.2	
Desired Residence Time (hr)	**0.5**	*30 minutes based on "Mixer Settler Time" Source
Known Flow Rate of Solid Out (lb/hr)	5,726	
Flow Rate of solid (g/hr)	2,597,476	
Flow Rate of Water Needed (L/hr)	4,078	
Volume of Solution in Reactor (L)	2,039	*Saying here that liquid level is half of the height of the reactor.This will give a hold-up time equal to the residence time.
Volume of Mixer (including solids) (ft^3)	247	
D (ft)	5.5	
L (ft)	10.5	*Solver sets volume calculated by specified by L and D to equal volume needed based on flow rate and residence time, by changing L.
Actual Volume (ft^3)	249	
Actual L/D	1.91	
Actual Volume (m^3)	**7.06**	*0.04 to 60 m^3
Reactor-Mixer/Settler for Adipic Acid (Design Textbook)		
K1	4.7116	
K2	0.4479	
K3	0.0004	
Volume (m^3)	7.06	0.04 to 60 m^3
logCp0	5.092	
Cp0	$ 123,647	
FBM (Reactor-Mixer Settler) - Table 4.7	4.0	
Cbm (2001)	$ 494,589	
Cbm (2016, using CEPCI of 545.1)	$ 674,610	
Utility Cost: Horsepower		
Volume of Fluid (1/2 of Volume calculated based on f	123.53	
Volume of Fluid (gallons)	924	
HP	1.386	

Table A.13.: Nylon Salt Agitated Reactor R-100 Sizing and Costing

NYLON SALT PREPARATION		
Jacketed Agitated Reactor: Preparing Nylon Salt Solution		
Desired Residence Time (hr)	**0.5**	*Use same as residence time as for mixers.
Known Volumetric Flow Rate of Adipic Acid (ft^3/hr)	**84.43**	
Known Volumetric Flow Rate of HMDA (ft^3/hr)	**103.07**	
Flow Rate of Water Added (L/hr)	47,956	
Flow Rate of Water Added (ft^3/hr)	1,693	
Total Volumetric Flow Rate in Reactor (ft^3/hr)	**1,881**	
Volume of Solution in Reactor (ft^3)	940.49	
Volume of Mixer (ft^3)	1,881	*Saying here that liquid level is half of the height of the reactor. This will give a hold-up time equal to the residence time.
D (ft)	11.0	
L (ft)	20	
Actual Volume (ft^3)	1,901	
Actual L/D	1.82	
Actual Volume (m^3)	**53.82**	*0.1 to 35 m^3
Reactor-Mixer/Settler for Adipic Acid (Design Textbook)		
K1	4.1052	
K2	0.532	
K3	-0.0005	
Volume (m^3)	53.82	
logCp0	5.025	
Cp0	$ 105,822	
FBM (Reactor) - Table 4.7	4.0	
Cbm (2001)	$ 423,288	
Cbm (2016, using CEPCI of 545.1)	$ 577,356	
Utility Cost: Horsepower		
Volume of Fluid (1/2 of Volume calculated based on fluid) (ft^3)	940.49	
Volume of Fluid (gallons)	7,035	
HP	10.553	

Table A.14.: Pump P-101 Sizing and Costing

Utilities	Power php, hp		26.83
Inlet Conditions:			
	℃	℉	
Temperature,	50		122
Pressure (psia)	90		
Outlet Conditions:			
	℃	℉	
Temperature,	50		122
Pressure (psia)	198.00		
P-101: Pump Sizing with an elvation change			
Sizing			
Inlet Flow Rate of salt solution (lbm/hr)	117392.49	Obtained from salt CSTR	
Salt density (lbm/ft3)	74.96	See Crystallizer body sizing	
Inlet Flow Rate of salt solution (gpm)	195.25	unit conversion	
Outlet pressure from salt CSTR (psia)	90.00	Obtained from Salt CSTR	
ΔP HEX (psi)	5.00		
Crystallizer pressure (psia)	191.00	from crystallizer	
ΔP Necessary (psia), +2 psi	108.00	$\Delta P_{pump}+\Delta P_{hydrostatic}+\Delta P_{losses}$	
ε_{pump}	0.51	Interpolated From Turton Table 11.9	
W_{pump} (hp)	24.15	Flow Rate*$\Delta P/\varepsilon_{pump}$	
ε_{driver}	0.9	Estimation from Turton 11.5, midpoint	
$W_{purchased}$ (hp)	26.83	$W_{pump}/\varepsilon_{driver}$	
$W_{purchased}$ (kW)	20.01	Unit conversion	
Costs:			
Purchased Equipment Costs			
Result	C^o_p	$	5,239.97
Variables/Info	Equipment Type	Pump	
	Equipment Description	Centrifugal	
(*unit)	Capacity: Shaft power (kW)		**20.01**
(to check)	min		1
	max		300
	K1		3.3892
	K2		0.0536
	K3		0.1538
Pressure Factors			
Result	Fp		1.20
Variables/Info	Equipment Type	Pump	
	Equipment Description	Centrifugal	
psia	Operating pressure		196.00
psia	Design pressure, P		246.00
(*barg)	Design pressure, P		15.95
(to check)	min		10
	max		100
	C1		-0.3935
	C2		0.3957
	C3		-0.00226
(*unit)	Diameter, D (m)		
Bare Module Cost			
Result	C_{BM}	$	32,820.83
	Equipment Type	Pump	
	Equipment Description	Centrifugal	
	MOC	SS	
	Identificaiton number		39
	F_M		2.7
	B1		1.89
	B2		1.35
Purchased Cost, C_p		$	23,308.54
Installed Cost, C_{BM}		**$**	**45,065**
Installation Cost		$	21,756.03
Year 2001	C.I.		397
Desired year (2016)	C.I.		545.1
Total cost including spare pump	**$ 90,129**		

Table A.15.: Heat Exchanger E-102 Sizing and Costing

E-102: Heat Exchanger (Fixed tube) (shell: steam and tube: nylon salt)			
Sizing:	ft^2	m^2	
Area	372.350	34.592	
Uo (Btu/hr*ft^2*°F)	150	(Heuristic from Turton for condensing steam)	
Temperatures	℃	°F	
Tcool,in	50	122	
Tcool,out	190	374	
Temperature approach	63.89		
Thot,in	253.89	489	high pressure steam
Thot,out	253.89	489	
Log Mean Temperature	102.87	217.16	
Correction Factor, F	1		
P	0.69		
R	0.00		
P'	0.69		
Heat Duty (Btu/hr)	1.21E+07		
Latent Heat (Btu/lbm)	728.852	high pressure steam	
Steam mhot (lbm/hr)	16641.2271	Utility cost	
Nylon Salt mcold (lbm/hr)	117392.49		
Heat Capacity of Nylon Salt (Btu/lbm*°F)	0.41	From encylcopedia	
Purchased Equipment Costs			
Result	C^o_p	$ 17,637	
Variables/Info	Equipment Type	HEX	
	Equipment Description	Fixed tube	
(*unit)	Area, m2	**35.0**	(in the range)
(to check)	min	10	
	max	1000	
	K1	4.3247	
	K2	-0.303	
	K3	0.1634	
Pressure Factors			
Result	Fp	1.19	
	Fp, process vessels		
Variables/Info	Equipment Type	HEX	
	Equipment Description	shell and tube	
	P nylon salt in	198.00	
psia	P steam in	614.70	
psia	Design pressure, P	664.70	
(*barg)	Design pressure, P	44.82	(in the rang)
(to check)	min	5	
	max	140	
	C1	0.03881	
	C2	-0.11272	
	C3	0.08183	
	Diameter, D		
Bare Module Cost			
Result	C_{BM}	$ 91,499.71	
	$C_{BM, process vessel}$		
	Equipment Type	HEX	
	Equipment Description	shell and tube	(salt in shell, steam in tube)
	MOC	CS shell / SS tube	(due to acid component)
	Identificaiton number	4	
	F_M	1.8	
	B1	1.63	
	B2	1.66	
Purchased Cost, Cp		$ 51,904.45	
Installed Cost, C_{BM}		**$ 125,633**	
Year 2001	C.I.	397	
Desired year (2016)	C.I.	545.1	

Table A.16.: Condenser E-103 Sizing and Costing

E-103: Condenser (Fixed tube) (water vapor in shell, C.W. in tube)			
Sizing:	ft^2	m^2	
Area	2141.807	198.980	
Uo (Btu/hr*ft^2*°F)	150	(Heuristic for condenser)	
Temperatures	℃	°F	
Tcool,in	30	86	(C.W. Heuristic from Turton, 30
Tcool,out	45	113	
Approach Temp.	160	320	
Thot,in	190	374	(Melting point of Nylon salt, see
Thot,out	190	374	
Log Mean Temperature	274.28		
Correction Factor, F	1		
P	0.09		
R	0.00		
P'	0.09		
Heat Duty (Btu/hr)	8.81E+07		
Latent Heat (Btu/lbm)	850.73	(at 190C, Steam table, Moran)	
Maximum amount of water can vaporize (lbm/hr)	116394.73		
Actual water vaporize mhot (lbm/hr)	103579	(calculated based on crystallizer sizing and Vmax of va	
C.W. flowrate (m3/hr)	3277.65	(For utilities cost)	
Density of C.W. (kg/m3)	995.72		
C.W. mcold (lbm/hr)	3.26E+06		
Heat Capacity of water (Btu/lbm*°F)	1	Properties spreadsheet	
Purchased Equipment Costs			
Result	C^o_p	$ 31,022.13	
Variables/Info	Equipment Type	HEX	
	Equipment Description	Fixed tube	
(*unit)	Area, m2	**199.0**	(in the range)
(to check)	min	10	
	max	1000	
	K1	4.3247	
	K2	-0.303	
	K3	0.1634	
Pressure Factors			
Result	Fp	1.05	
	Fp, process vessels		
Variables/Info	Equipment Type	HEX	
	Equipment Description	Fixed tube	
psia	P C.W. assume	100	
C	T water vapor	190	
psia	P condenser (water vapor P)	181.368	(Sat. steam table, Moran)
psia	Design pressure, P	231.37	
(*barg)	Design pressure, P	14.94	(in the range)
(to check)	min	5	
	max	140	
	C1	0.03881	
	C2	-0.11272	
	C3	0.08183	
	Diameter, D		
Bare Module Cost			
Result	C_{BM}	$ 195,920.87	
	$C_{BM, process\ vessel}$		
	Equipment Type	HEX	
	Equipment Description	shell and tube	(water vapor in shell, C.W. in tul
	MOC	SS	
	Identificaiton number	5	
	F_M	2.7	
	B1	1.63	
	B2	1.66	
Purchased Cost, Cp		$ 120,228.36	
Installed Cost, C_{BM}		**$ 269,009**	
Year 2001	C.I.	397	
Desired year (2016)	C.I.	545.1	

Table A.17.: Crystallizer R-101 Sizing and Costing

R-100: Crystallizer Body			
Sizing:			
Volume required	Volume required (m3)	20.90	(<"crystallizer volume", satisfied
	Voume required (ft3)	738.25	
	Nylon salt M.w. (lbm/lbmol)	262.35	
	Water M.w. (lbm/lbmol)	18.00	
	Production Rate (lbm/hr)	13813.49	
	Retention hour (hr)	3.38	(Heuristic for forced-circulation
	Nylon salt density (lbm/ft3)	74.96	(Source: http://allinno.com/m/p
	Water density (lbm/ft3)	54.69	
	Concentration of solids (%)	50	
	Slurry density (lbm/ft3)	63.24	(Source: Slurry density calculatic
Maximum vapor velocity	Vmax (m/s)	0.29	
	Vmax (ft/s)	0.94	
	constant C (ft/s)	0.08	(recommended for vapor heads
	Operating temperature (℃)	190	
	Operating temperature (℉)	374	
	Liq. density of water (lbm/ft3)	54.69	0.0011414
	Vap. density of water (lbm/ft3)	0.40	0.1565
Minimum Cross-sectional area	Cross-sectional area (m2)	0.95	(<"evaporator area", satisfied)
	Cross-sectional area (ft2)	10.27	(This value is not controlling)
Crystallizer Volume	Total volume (m3)	40.75	
	Diameter (m)	3.2	(Heuristic)
	Liquid level (m)	4	(Heuristic)
	Cone volume (m3)	8.58	
	Straight side (m3)	32.17	
	Diameter (ft)	10.50	
	Length (ft)	13.12	
	Cone volume (ft3)	302.72	
	Straight side (ft3)	1135.20	
	Total volume (ft3)	1437.92	
Evaporator area (m2) (for costing)	Area (m2)	8.04	
	Area (ft2)	86.52	
Costs:			
Purchased Equipment Costs			
Result	C^o_p	$ 262,671.50	
Variables/Info	Equipment Type	Evaporators	
	Equipment Description	Forced-circulation (pumped)	
(*unit)	Capacity (m2)	**9.00**	(in the range)
(to check)	min	5	
	max	1000	
	K1	5.0238	
	K2	0.3475	
	K3	0.0703	
Pressure Factors			
Result	Fp	1.00	
	Fp, process vessels	0.50	
Variables/Info	Equipment Type	Evaporator	
	Equipment Description	Forced-circulation (pumped)	
℃	Operating temp.	190	(Operating temp. heuristic chec
psia	P condenser	181.37	(Antoine equation) (Need to be
psi	ΔP return line	2	
psi	ΔP hydrostatic	6.83	$\Delta P_{hydrostatic} = \rho_{Nylon\ salt}$
psia	P bot	190.20	
psia	Design pressure, P	240.20	
(*barg)	Design pressure, P	15.55	
(to check)	min	0	
	max	0	if 10 < p (barg) < 150
	C1	0	0.1578
	C2	0.00	-0.2992
	C3	0	0.1413
(*unit)	Diameter, D (m)		
Bare Module Cost			
Result	C_{BM}	$ 1,024,418.86	
	Equipment Type	2	
	Equipment Description	vertical	
	MOC	SS	
	Identificaiton number	26	
	F_{BM}	3.9	
Purchased Cost, $C_{p\ Evaporator}$		$ 703,288.06	
Installed Cost, $C_{BM\ Evaporator}$		**$ 1,406,576**	
Installation Cost		$ 703,288.06	
Year 2001	C.I.	397	
Desired year (2016)	C.I.	545.1	

Table A.18.: Pump P-102 Sizing and Costing

Utilities	Power php, hp		2.96
Inlet Conditions:			
	℃	℉	
Temperature,	190		374
Pressure (psia)	191.00		
Outlet Conditions:			
	℃	℉	
Temperature,	190		374
Pressure (psia)	259.00		
P-102: Pump Sizing with an elvation change			
Sizing			
Inlet Flow Rate of salt slurry (lbm/hr)	13813.49	Obtained from Crystalllizer	
Salt slurry density (lbm/ft3)	63.24	See Crystallizer body sizing	
Inlet Flow Rate of salt slurry (gpm)	27.23	unit conversion	
Outlet pressure from crystalizer (psia)	191.00	Obtained from Crystalllizer	
Reactor pressure (psia)	250.00	from polymerization reactor	
Height of reactor (m)	4.69	From polymerization reactor	
Height of reactor (ft)	15.40	Unit conversion	
ΔP hydrostatic (psi)	6.76		
ΔP Necessary (psia), +2 psi	67.76	$\Delta P_{pump}+\Delta P_{hydrostatic}+\Delta P_{losses}$	
ε_{pump}	0.40	Interpolated From Turton Table 11.9	
W_{pump} (hp)	2.66	Flow Rate*$\Delta P/\varepsilon_{pump}$	
ε_{driver}	0.9	Estimation from Turton 11.5, midpoint	
$W_{purchased}$ (hp)	2.96	$W_{pump}/\varepsilon_{driver}$	
$W_{purchased}$ (kW)	2.21	Unit conversion	
Costs:			
Purchased Equipment Costs			
Result	C^o_p	$	2,665.33
Variables/Info	Equipment Type	Pump	
	Equipment Description	Centrifugal	
(*unit)	Capacity: Shaft power (kW)		**2.21**
(to check)	min		1
	max		300
	K1		3.3892
	K2		0.0536
	K3		0.1538
Pressure Factors			
Result	Fp		1.31
Variables/Info	Equipment Type	Pump	
	Equipment Description	Centrifugal	
psia	Operating pressure		256.76
psia	Design pressure, P		306.76
(*barg)	Design pressure, P		20.14
(to check)	min		10
	max		100
	C1		-0.3935
	C2		0.3957
	C3		-0.00226
(*unit)	Diameter, D (m)		
Bare Module Cost			
Result	C_{BM}	$	17,804.73
	Equipment Type	Pump	
	Equipment Description	Centrifugal	
	MOC	SS	
	Identificaiton number		39
	F_M		2.7
	B1		1.89
	B2		1.35
Purchased Cost, C_p		$	12,985.23
Installed Cost, C_{BM}		**$**	**24,447**
Installation Cost		$	11,461.53
Year 2001	C.I.		397
Desired year (2016)	C.I.		545.1
Total cost including spare pump	**$ 48,894**		

Table A.19.: Polymerization Reactor R-102 Sizing and Costing [47]

Polymerization Reactor (CSTR)									
		Mass Flowrate (lbm/hr)							
		Inlet		Generated		Outlet		Accumulation	
Component:	Nylon salt (1:1 molar ratio)	12926.43	Nylon 6 6	8183.35	Nylon 6 6	10213.88	Nylon 6 6	-2030.53	
	amine end-group	5726.46	amine end-group	-4201.60	amine end-group	482.32	amine end-group	1042.54	
Unit conversion from g to lbm	carbonxyl end-group	7199.97	carbonxyl end-group	-5282.73	carbonxyl end-group	606.43	carbonxyl end-group	1310.80	
453.59237	water	887.06	Water	650.85	Water	1699.81	Water	-161.90	IOGA
	To check M.B.	13813.49		-650.13		13002.44		160.91	0.00
Utility	Dowtherm A (Jacketed) (lbm/hr)	674.61				0.78553556			
	Cooling water (m3/hr)	60.58				0.08373479			
	Cooling water (lbm/hr)	6.03E+04							
	Power (Agitation) (hp)	24.16	(Heuristic from Seider, 0.5-1.5/1000gal, 3 times when heat is to be transfered)						
	duty (thermal system) (GJ/hr)	0.78							
Feed Conditions:									
	℃	℉							
Temperature,	190	374	(assume, and also depends on what comes out of the evaporator)						
Pressure (psia)	252.00		(lower than vapor pressure)						
Operating conditions:									
	℃	℉							
Temperature, operating	268.13	514.63							
Pressure (psia), operating	250.00	(literature, brydson-plastic materials	(lower than the vapor pressure, but higher than the minimum pressure in literature range, Ogata: 15-20 kg/cm2)						
Pressure (psia), vapor pressure	783.05								
Outlet conditions of Nylon 6,6									
	℃	℉							
Temperature	268.13	514.63							
Pressure (psia)	250.00	(literature, brydson-plastic materials							
Outlet conditions of Water vaporize									
	℃	℉							
Temperature	204.83	400.69	Phase: liquid						
Pressure (psia)	243.00								
Desired product (Nylon 6,6) quality									
Instantaneous Yield	1								
Overall Yield	1.00								
Number-average degree of polymerization	11.87	(source of equation used: Fogler-polymerization examples, website)							
Number-average molecular weight (g/mol)	2687.02	(lower than the range due to p lower than 0.99, expected 12000-20000 for p > 0.99)							

Table A.19.: Polymerization Reactor R-102 Sizing and Costing (continued)

	CSTR, Dowtherm Jacketed			
Sizing:				
CRE Algorithm (CSTR)	Rev.,single rxn	A + C ⇋ L + W	**(Heuristic also supports the choice of CSTR since feed co**	
Components convention	a	amine end-group		
	c	carbonxyl end-group		
	l	nylon 6,6 (polymer)		
	w	water molecule		
Design specification				
Outlet Nylon 6,6 given	Fl (lbm/year)	8.50E+07		
	M.W of l (g/mol)	226.32		
	density of l (g/m3)	1140000		
	Fl (mol/s)	5.69	(assume a service factor of 0.95)	
	ml (g/s)	1286.93		
Reactor size	reactor volume V (m3)	81.24		
	reactor volume V (ft3)	779.11		
	product polymer volume V (gal)	5367.95	(Used to calculate power input for OPERATING COST later	
	product polymer volume V (m3)	20.32	(assume height is double liquid level, diameter equal liqui	
	liquid level (m)	2.35		
	diameter (m)	2.35		
	height (m)	4.69		
	wall thickness (m)	0.47	(thickness less than 1/4*D, Turton A.2.1)	
	liquid level (ft)	7.70	(Round up to the nearest 1/2 ft)	
8	diameter (ft)	7.70		
15.5	height (ft)	15.40		
	wall thickness (ft)	1.54		
Other (OPTIMIZATION VARIABLE)	spacetime (s)	18000	(use 5 hours, referenced from Ogata, heuristic from Fogle	
	fraction of a, p	0.92	(Might be able to use for optimization, see Polymerizatior	
Initial condition	To (K)	463		
(lbm/lbmol) (for amine end-group)	M.W. of HMDA	116.2		
(lbm/lbmol) (for carbonxyl end-group)	M.W. of Adipic acid	146.1		
	Fao (mol/s)	6.21	(Update from POLYMATH)	
	Fco (mol/s)	6.21	(stoichiometric equivalent)	
	Flo (mol/s)	0		
	Fwo (mol/s)	6.21		
	Cao (mol/m3)	5500.40		
	Cco (mol/m3)	5500.40		
	Clo (mol/m3)	0		
	Cwo (mol/m3)	5500.40	1	
	vo (m3/s)	1.13E-03	(assume density change is negligible, might not be applie	
Stoichiometry	(Results from Polymath Report)			
Concentration (mol/m3)	Ca	463.2833		
	Cc	463.2833		
	Cl	5037.561	5037.12	
	Cw	10540		
	Ct	16504.1276		
Molar flowrate (mol/s)	Fa	0.52		
	Fc	0.52		
	Fl	5.69	(check with Fl above)	
	Fw	11.90		
Mole fraction	xa	0.03		
	xc	0.03		
	xl	0.31		
	xw	0.64		
Relative Rate	ra (mol/m3.s)	-0.22		
	rc (mol/m3.s)	-0.22		
	rl (mol/m3.s)	0.22		
	rw (mol/m3.s)	0.22		
Rate Law (Steppan article)	forward ko (1/hr)	8.25		
	equilibrium Ko	304.26		
	deltaHo (cal/mol)	-4204.03		
	deltaHo (J/mol)	-17589.68		
	activ. energy (kcal/mol)	21.40	(Steppan)	
	gas constant (kcal/mol.K)	0.001987		
	Ref. Temp. Tr (K)	473.00	(200 degree C)	
	forward k (1/hr)	145.06		
	equilibrium K	173.25		
	rw (mol/m3.s)	0.22		

Table A.19.: Polymerization Reactor R-102 Sizing and Costing (continued)

Energy Balance				
Rxn	T (K) (Polymath)	541.125	POLYMATH	
	T ℃	268.125	(expected 200-265C)	
	Cpa (J/mol.K)	68.14	Check "chemical properties from perry" spreadsheet	
	Cpc (J/mol.K)	275.37		
	Cpl (J/mol.K)	377.92		(range 200-220℃, Ogata)
	Cpw (J/mol.K)	75.4		
(J/mol)	deltaHrxn (J/mol)	-10108.87	(-deltaHrxn >0: exothermic)	
Medium fluid: Dowtherm	Ta supply (℃)	300		
	Ta supply (K)	573		
	ΔT approach (K)	10	(minimum temperature approach of 10C , Turton heuristi	
	Ta return (K)	551.125		
(J/g.K)	Cp dowtherm	2.3	(Engineering toolbox and Dowtherm a properties online s	
Heat duty info	Q (J/s=W)	-6.28E+04	(Turton chapter 19, 3rd ed.)	$Q = Fao * DeltaH$
	A (m2)	34.62		
	U (J/m2.s.K)	280	(Heuristic estimation, liquid to liquid for dowtherm,Turto	
	UA (J/s.K)	9694.81		
Utility cost of Dowtherm A	Dowtherm flowrate (gal/min)	85.00	(at normal operating condition, pp. 760 Turton 4th editio	
	Dowtherm density (kg/m3)	800.00		
	Dowtherm flowrate (g/s)	4290.13	(at 300 degree C, Engineering toolbox)	
	Downtherm flowrate (lbm/hr)	34049.22795		
	Process heating duty (W)	2.16E+05		
Costs:				
Purchased Equipment Costs				
Result	C^o_p	$ 131,634.44		
Variables/Info	Equipment Type	Reactors		
	Equipment Description	Jacketed agitated	53	
(*unit)	Capacity (m3)	**81.24**	(in the range)	
(to check)	min	0.1		
	max	35		
	K1	4.1052		
	K2	0.532		
	K3	-0.0005		
Installed Cost, $C_{BM,reactor}$		**$ 722,962**	(not follow process vessel, using heuristic Fbm)	
Year 2001	C.I.	397		
Desired year (2016)	C.I.	545.1		

Table A.20.: Condenser E-104 Sizing and Costing

E-104: Condenser (Double pipe) (water vapor in shell, C.W. in tube)				
Sizing:	ft^2		m^2		
Area	30.592		2.842	
Uo (Btu/hr*ft^2*°F)	150	(Heuristic for condenser, Turton)		
Temperatures	℃		°F	
Tcool,in	30		86	
Tcool,out	45		113	
Temperatures approach	10		50	(based on temperture differen
Thot,in (water vapor)	268.125		514.625	
T sat. Vap. At 250 psia	204.829		400.6922	
Thot,out	204.829		400.6922	
Log Mean Temperature			356.39	
Correction Factor, F	1.00			
P	0.06			
R	4.22			
P'	0.06			
Heat Duty (Btu/hr)	1.63E+06			
Water vaporize mhot (lbm/hr)	1699.81			
Latent heat (Btu/lbm)	826.05	(at 250psia, 204.829C)		
C.W. flowrate (m3/hr)	60.58	(For utilities cost)		
Density of C.W. (kg/m3)	995.72			
C.W. mcold (lbm/hr)	60324.65			
Heat Capacity of water vapor (Btu/lbm*°F)	1.16	Engineering toolbox, at 250C		
Heat Capacity of C.W (Btu/lbm*°F)	1	Engineering toolbox, at 30C		
Purchased Equipment Costs				
Result	C^o_p	$	2,914.91	
Variables/Info	Equipment Type	HEX		
	Equipment Description	Fixed tube		
(*unit)	Area, m2		**3.0**	(out of range)
(to check)	min		1	
	max		10	
	K1		3.3444	
	K2		0.2745	
	K3		-0.0472	
Pressure Factors				
Result	Fp		0.96	
	Fp, process vessels			
Variables/Info	Equipment Type	HEX		
	Equipment Description	Double pipe		
C	T top		268.125	P condenser (P water vapor)
psia	P reactor		250.00	
psi	ΔP return line		2.00	
psia	Pcondenser		248.00	
psia	Design pressure, P		298.00	
(*barg)	Design pressure, P		19.53	(in the range)
(to check)	min		40	
	max		100	
	C1		0.6072	
	C2		-0.912	
	C3		0.3327	
	Diameter, D			
Bare Module Cost				
Result	C_{BM}	$	16,838.40	
	$C_{BM,\ process\ vessel}$			
	Equipment Type	HEX		
	Equipment Description	shell and tube		
	MOC	SS		
	Identificaiton number		5	
	F_M		2.7	
	B1		1.74	
	B2		1.55	
Purchased Cost, Cp		$	10,423.17	
Installed Cost, C_{BM}		**$**	**23,120**	
Year 2001	C.I.		397	
Desired year (2016)	C.I.		545.1	

Table A.21.: Dowtherm Boiler H-100 Sizing and Costing

Dowtherm Boiler for the reactor- Diphenyl Heater				
Costing:				
Purchased Equipment Costs				
Result	C^o_p	$	18,508.26	
Variables/Info	Equipment Type	Heaters		
	Equipment Description	Diphenyl heater		
(*unit)	Duty, kW		**215.8**	(not in the range)
(to check)	min		650	
	max		10750	
	K1		2.2628	
	K2		0.8581	
	K3		0.0003	
Pressure Factors				
Result	Fp		1.09	
	Fp, process vessels			
Variables/Info	Equipment Type	Heater		
	Equipment Description	Diphenyl heater		
psia	P		152.70	(min.operating pressure at 40(
psia	Design pressure, P		202.70	
(*barg)	Design pressure, P		12.96	(in the range)
(to check)	min		2	
	max		200	
	C1		-0.01633	
	C2		0.056875	
	C3		-0.00876	
	Diameter, D			
Bare Module Cost				
Result	C_{BM}	$	44,248.28	
	Equipment Type	Heater		
	Equipment Description	Diphenyl-based oil		
	MOC	N/A		
	Identificaiton number		56	
	F_{BM}		2.2	
Purchased Cost, Cp		$	60,755.01	
Installed Cost, C_{BM}		**$**	**60,755**	
Year 2001	C.I.		397	
Desired year (2016)	C.I.		545.1	

Table A.22.: Pump P-103 Sizing and Costing

Pumping Molten Nylon 66		
Utilities	Power php, hp	24.14
Inlet Conditions:		
	℃	℉
Temperature,	268.13	515
Pressure (psia)	250.00	
Outlet Conditions:		
	℃	℉
Temperature,	268.13	515
Pressure (psia)	1002.00	
P-103: Pump Sizing with an elvation change		
Sizing		
Inlet Flow Rate of molten nylon 66 (lbm/hr)	11302.64	Obtained from Polymerization CSTR
Nylon 6,6 density (lbm/ft3)	71.17	Obtained from Polymerization CSTR
Inlet Flow Rate of salt slurry (gpm)	19.80	unit conversion
Outlet pressure from CSTR (psia)	250	Obtained from Crystalllizer
Extruder pressure (psia)	1000	Jessica group
ΔP Necessary (psia), +2 psi	752	$\Delta P_{pump}+\Delta P_{hydrostatic}+\Delta P_{losses}$
ε_{pump}	0.40	Interpolated From Turton Table 11.9
W_{pump} (hp)	21.72	Flow Rate*$\Delta P/\varepsilon_{pump}$
ε_{driver}	0.9	Estimation from Turton 11.5, midpoint
$W_{purchased}$ (hp)	24.14	$W_{pump}/\varepsilon_{driver}$
$W_{purchased}$ (kW)	18.00	Unit conversion
Costs:		
Purchased Equipment Costs		
Result	C^o_p	$ 28,749.92
Variables/Info	Equipment Type	Pump
	Equipment Description	Reciprocating
(*unit)	Capacity: Shaft power (kW)	**18.00**
(to check)	min	0.1
	max	200
	K1	3.8696
	K2	0.3161
	K3	0.122
Pressure Factors		
Result	Fp	1.54
Variables/Info	Equipment Type	Pump
	Equipment Description	Reciprocating
psia	Operating pressure	1000.00
psia	Design pressure, P	1050.00
(*barg)	Design pressure, P	71.38
(to check)	min	10
	max	100
	C1	-0.245382
	C2	0.259016
	C3	-0.01363
(*unit)	Diameter, D (m)	
Bare Module Cost		
Result	C_{BM}	$ 197,912.10
	Equipment Type	Pump
	Equipment Description	Reciprocating
	MOC	SS
	Identificaiton number	28
	F_M	2.4
	B1	1.89
	B2	1.35
Purchased Cost, C_p		$ 146,025.92
Installed Cost, C_{BM}		**$ 271,743**
Installation Cost		$ 125,716.85
Year 2001	C.I.	397
Desired year (2016)	C.I.	545.1
Total cost including spare pump	**$ 543,486**	

Table A.23: Extruder MP-102 Sizing and Costing

Extruder		
Standard Extruder Equations		Comments (use Standard Extruder Equations)
Screw Diameter (m)	0.20	
Screw Diameter (ft)	0.67	
Screw Diameter (in)	8	From website with "handy outputs"
Total Length (m)	6.096	20-30D-Chose 25; page 307 also
Total Length (ft)	20.0	
Length of Feed Section (m)	1.6256	4-8D-chose 8
Length of Feed Section (ft)	5.33	
Length of metering section (m)	2.032	6-10D-chose 10
Length of metering section (ft)	6.66	
Number of Parallel Flights	1	
Flight Pitch	0.2032	helix angle 17.66 degrees
Flight Width (m)	0.02032	
Channel Depth in feed section (m)	0.03556	0.15-0.2D-chose 0.175
Channel Depth Ratio	3	2-4, chose 3
Compression Length (m)	0.406	Page 306-2.5:1 and 2D in "Extruder Equations" page 628
Compression Length (ft)	1.33	
L/D	30	Total Length/Diameter
RPM	100	From website with "handy outputs"
Output (lb/hr)	5200	From website with "handy outputs"
Costing:		Example in Book-Page 433; extruders for polymers (excluding drive and motor); FOB varies by +/- 30%
FOB	$76,262.88	$70,000
L+M*	1	
L+M Cost	$ 76,262.88	
Physical Module Cost, PM	$ 91,515.46	Use L+M cost plus 15-25% of FOB-chose 20%
Bare Module Cost, BM	$ 99,141.75	use PM plus 10-45% of L+M cost-chose 10%
CEPCI (1957-1959)	1000	
CEPCI (2017)	545.1	
Cbm (2017)	$ 54,042.17	
Drive Power (kW)	12.0	10
n		0.47
L/M		0.27
Alloy Cost Factors		
-c/s		1
-s/s		1.19
-monel		1.4
Variable Speed Drive Factor		1.5
L/D	30	

Table A.23.: Extruder MP-102 Sizing and Costing (ctn)

Drive				
Sizing:			**Cbm (Drive and Motor)**	$7,089
Power (kW)	12		**Cbm (Extruder)**	$54,042
Power (hp)	16		**Total Extruder Cost**	$61,131
Costing:				
K1	1.956	Totally Enclosed, Electric		
K2	1.7142			
K3	-0.2282			
Shaft Power (kW)	12			
logCp0	3.54016			
Cp0	3468.67			
Installed Cost:				
Identification Number	14			
Fbm	1.5			
B1	1.63			
B2	1.66			
Cbm (2001)	$5,203			
Cbm (2016)	$7,089			

Table A.24.: Condenser E-105 Sizing and Costing

Condenser during casting wheel		
Utilities		
	C.W. (lbm/hr)	7.51E+04
E-105: Condenser (Fixed tube) (C.W. in tube, steam in shell)		
Sizing:	ft^2	m^2
Area	120.817	11.224
Uo (Btu/hr*ft^2*°F)	150	(Heuristic for condenser)
Temperatures	℃	°F
Tcool,in	30	86
Tcool,out	45	113
Approach Temp.	70.00	158
Thot,in	100.00	212
Thot,out	100.00	212
Log Mean Temperature	111.96	
Correction Factor, F	1	
P	0.21	
R	0.00	
P'	0.21	
Heat Duty (Btu/hr)	2.03E+06	
Latent Heat (Btu/lbm)	970.34	(at 100C, Steam table, Mor
water vaporize mhot (lbm/hr)	2091	Jessica
C.W. mcold (lbm/hr)	7.51E+04	
Heat Capacity of water (Btu/lbm*°F)	1	Properties spreadsheet
Purchased Equipment Costs		
Result	C^o_p	$ 15,417.32
Variables/Info	Equipment Type	HEX
	Equipment Description	Fixed tube
(*unit)	Area, m2	**12.0**
(to check)	min	10
	max	1000
	K1	4.3247
	K2	-0.303
	K3	0.1634
Pressure Factors		
Result	Fp	1.01
	Fp, process vessels	
Variables/Info	Equipment Type	HEX
	Equipment Description	Fixed tube
C	T water vapor	100.00
psia	P condenser (water vapor P)	14.778
psia	P C.W. (assumption)	100.000
psia	Design pressure, P	150.00
(*barg)	Design pressure, P	9.33
(to check)	min	5
	max	140
	C1	0.03881
	C2	-0.11272
	C3	0.08183
	Diameter, D	
Bare Module Cost		
Result	C_{BM}	$ 95,265.72
	$C_{BM, process vessel}$	
	Equipment Type	HEX
	Equipment Description	shell and tube
	MOC	SS
	Identificaiton number	5
	F_M	2.7
	B1	1.63
	B2	1.66
Purchased Cost, Cp		$ 58,011.67
Installed Cost, C_{BM}		**$ 130,804**
Year 2001	C.I.	397
Desired year (2016)	C.I.	545.1

Table A.25.: Casting Wheel MP-103 Sizing and Costing

Casting Wheel		
Sizing:		
Diameter (ft)	16.4	
Diameter (m)	5	4 to 8 m; "Scattering Methods and the Properties..." article
Height (m)	1.5	1.2-1.5m
Height (ft)	4.92	
Volume (m^3)	29.5	
Volume (ft^3)	1039.3	
Pressure (psi)	14.7	
Circumference of the wheel (m)	31.42	
Circumference (ft)	103.04	50-150
Speed (m/min)	150	
Speed (rpm)	4.77	
Costing:		
K1	3.5565	
K2	0.3776	
K3	0.0905	
Volume (m^3)	29	
logCp0	4.30656783	
Cp0	20256.65959	
C1	0	
C2	0	
C3	0	
P operating (psi)	14.70	
P Design (barg)	3.45	
Fp	2.5828	
Purchase Cost:		
Identification Number	1	
Fm	1.7	stainless steel coating
Cp (2001)	$88,943	
Cp (2017)	$122,122	
Installed Cost:		
Identification Number	14	
B1	1.49	
B2	1.52	
Cbm (2001)	$165,375	
Cbm (2017)	$227,068	
Installation Cost	$104,946	

Temperature in (°F)	530.6	514.6 full capacity
Temperature Out (°F)	257	125 C
Pressure (psi)	14.7	
Heat Capcity of Nylon 6,6 (J/kg*K)	0.00167	
Heat Capacity (Btu/lb*F)	0.3343844	
Heat Duty of Nylon (Btu/hr)	626077	
Mass Flowrate of Nylon 6,6 (lb/hr)	6843.3	11302 for full capacity
Mass Flowrate of Cooling water on outside of wheel (lb/hr)	645	value for 67% case
Heat Capacity of Water (Btu/lb*F)	0.997	
Mass Flowrate of cooling water inside the wheel (lb/hr)	25	
Thermal Conductivity of Stainless Steel (Btu*in/hr*ft^2*°F)	132	
Wheel Temperature outside (°F)	530.6	514.6 full capacity
Wheel Temperature inside (°F)	257	
Wall thickness of Casting Wheel (in)	6	
Cooling Water Temperature (°F)	86	
Cooling Water Pressure (psi)	100	need source
Area of Drum (m^2)	19.63	
Area of Drum (ft^2)	1.82	
Steam Exit Temperature (F)	212	steam table at 14.7; chE thermo book
Heat of Vaporization (Btu/lb)	970.3	

Drive	
Sizing:	
Power (kW)	75
	100.6 hp
Costing:	
K1	1.956
K2	1.7142
K3	-0.2282
Power (kW)	75
logCp0	4.367911966
Cp0	23329.85103
Installed Cost:	
Identification Number	14
Fbm	1.5
B1	1.63
B2	1.66
Cbm (2001)	$34,995
Cbm (2017)	$48,050
Casting Wheel (2017)	$227,068
Drive (2017)	$48,050
Total Casting Machine Cost (2017)	$275,117

Table A.26.: Chopper MP-104 Sizing and Costing

Chopper:		
Sizing:		
Rotor Speed (RPM)	3000	Retsch Example
Mass Flowrate (lb/hr)	10214	
Chopping Time (seconds)	60	
Time (hours)	0.017	
Mass (lb)	170.2	
Density (lb/ft^3)	71.1	
Volume (ft^3)	2.39	
Width (m)	1.5	
Width (ft)	4.92	
Length (ft)	3	Assume 3 feet
Area (ft^2)	14.76	
Area(m^2)	1.37	
Costing:	blender kneader	
K1	5.0141	
K2	0.5867	
K3	0.3224	
Area (m^2)	1.37	
logCp0	5.100757678	
Cp0	126112.3672	
P operating (psi)	14.70	
P Design (barg)	3.45	
Fp	1.1248	
Installed Cost:		
Fbm	1.12	
Cbm (2001)	$141,246	
Cbm (2017)	$193,937	

Drive:	
Sizing:	
Power (kW)	75
Power (hp)	100.6
Costing:	
K1	1.956
K2	1.7142
K3	-0.2282
Power (kW)	75
logCp0	4.367911966
Cp0	23329.85103
Installed Cost:	
Identification Number	14
Fbm	1.5
B1	1.63
B2	1.66
Cbm (2001)	$34,995
Cbm (2017)	$48,050

Total Cost of Chopper:	
Chopper (2017)	$193,937
Drive (2017)	$48,050
Total Chopper Cost (2017)	$241,987

Table A.27.: Dryer MP-105 Sizing and Costing

Dryer			**Drive**	
Type:	Horizontal Paddle Vacuum	should be jacketed and have a temp sensor to control temperature and therefore humidity		
Throughput available	< 30 – 1,000 lb./hr		**Sizing:**	
Sizing:		up to 30,000 lb/hr	Installed Power (kW)	90
Screw Diameter (mm)	2200			120.7 hp
Screw Diameter (ft)	7.22		**Costing:**	Drive with 90 kW
Length (mm)	6000		Power (kW)	90
Length (m)	6		**Costing:**	
Length (ft)	19.7		K1	1.956
Volume (ft^3)	22		K2	1.7142
Volume (ft^3)	776		K3	-0.2282
Area (m^2)	3.67		Power (kW)	90
Area (ft^2)	39.4		logCp0	4.434452154
Agitator Speed (RPM)	6		Cp0	27193
Pressure	14.7			
Temperature (°F)	180	Dryer temp source	Installed Cost:	
Pressure drop (psi)	5		Identification Number	14
			Fbm	1.5
			B1	1.63
Costing:	Drum Dryer		B2	1.66
K1	4.45742		Cbm (2001)	$40,789
K2	0.2731		**Cbm (2017)**	$56,005
K3	0.134			
Area (ft^2)	4		Dryer Cbm (2017)	$99,082
logCp0	4.654188429		Drive Cbm (2017)	$56,005
Cp0	45101.23443		**Total Dryer Cbm (2017)**	$155,087
Installed Cost:				
Fbm	1.6			
Cbm (2001)	$72,162			
Cbm (2017)	$99,082			

Table A.28.: Nylon Granule Storage Hopper TK-104 Sizing and Costing

Nylon 6,6 Pellet Storage Tank (Hopper)	
Sizing:	
Mass Flowrate (lb/hr)	6843.3
Time (hr)	96
Mass (lb)	656956.8
Density (g/cm^3)	1.14
Density (lb/ft^3)	71.1
Volume (ft^3)	9235
Volume (m^3)	261
Volume (m^3)	390.0
Temperature (°F)	158
Pressure (psi)	9.7
Diameter (m)	4.99
Diameter (ft)	16.4
Height (m)	20.0
Height (ft)	65.5
L/D	4
Volume (ft^3)	13787
Volume (m^3)	390
Costs:	Vertical Process Vessel
K1	3.4974
K2	0.4485
K3	0.1074
Volume (m^3)	390
logCp0	5.380534813
Cp0	240178.8787
P operating (psi)	9.70
P Design (barg)	3.10
Fp	2.4176
Purchase Cost:	
Identification Number	18
Fm	1
Cp (2001)	$580,660
Cp (2017)	$797,274
Installed Cost:	
Identification Number	14
B1	2.25
B2	1.82
Cbm (2001)	$1,597,204
Cbm (2017)	$2,193,037
Installation Cost	$1,395,763

POLYMATH Attachments:

Polymath Coding of the Chemical Reaction Engineering Algorithm Modeling Using Polymath for Autoclave (Polymerization reactor) as a CSTR

```
#Components: a-amine end-group, c-carbonxyl end-group, l-amide linkage (nylon 6,6), w-water molecule

#DESIGN SPECIFICATION AND INITIAL CONDITION
#Ml =85E6                                     #lbm/year
#MWl = 226.3                                  #g/mol, polymer data handbook
#densityl = 1140000                           #g/m3
Fl = 5.69                                     #mol/s, calculated, 0.95 service factor
#ml = 1286.93                                 #g/s
tau =  18000                                  #in sec, Ogata 5 hours residence time,
Fogler: 10min-4hour for industrial CSTR
To = 190+273                                  #Ogata, range 200-220C
Ta = 573                                      #K, Dowtherm a, maximum 400 degree
C, Turton heuristic
#T = 520                                      #K
#Ts = 550
V = Fl*226.3/1140000*tau                      #m3
A = 2*3.14*((2*V/3.14)^(1/3))^2               #m2, D=L, H=2L
U = 280                                       #J/m2.s.K, Heuristic
vo = V/tau                                    #m3/s
p = 1-Ca/Cao                                  # fraction of functional group amine (a),
MIGHT be able to use for optimization,

#Fao = Fa/(1-p)
Fao = (0-Fl)/(-rl)*(-ra)+Fa
Fco = Fao
Fwo = Fao                                     #use molar ratio from Ogata: range 0.5-
10 : salt/water

#Flo = 0
Cao = Fao/vo                                  #mol/m3
Cco = Fao/vo                                  #assuming Fao=Fco, due to
stoichiometric equivalence
Cwo = Fwo/vo


#MOLE BALANCE (single reaction, single phase, reversible, CSTR)
f(Ca) = vo*Cao-vo*Ca+ra*V
Ca(0) = 0.000001
f(Cc) = vo*Cco-vo*Cc+rc*V
Cc(0) =0.00001
f(Cl) = -vo*Cl+rl*V
Cl(0) = 2000
f(Cw) = vo*Cwo-vo*Cw+rw*V
Cw(0) = 10000

#RATE LAW (activate if reversible, homogeneous rxn)
rw = Ct*k/3600*(xa*xc-xl*xw/K)
        #Steppan and Giudici, r in mol/m3.s

        #rw is positive due to water being product
```

Polymath Coding of the Chemical Reaction Engineering Algorithm Modeling Using Polymath for Autoclave (Polymerization reactor) as a CSTR (continued)

```
k = ko *exp(E/R*(1/Tr-1/T))
          #1/hr, Arrhenius equation at a convenient Temp. Tr=200C
K = Ko *exp(deltaHo*10^(-3)/R*(1/Tr-1/T))
                    #literature used: Steppan

ko = exp(2.55-0.45*tanh(25*(xw-0.55)))+8.58*(tanh(50*(xw-0.10))-1)*(1-30.05*xc)
          #ko[=]1/hr; ko,Ko and detaHo models from Steppan
Ko = exp((1-0.47*exp(-xw^(1/2)/0.2))*(8.45-4.2*xw))
deltaHo = 7650*tanh(6.5*(xw-0.52))+6500*exp(-xw/0.065)-800
          #cal/mol, convert to J/mol: multiply 4.184
Tr = 473
          #in K, Steppan
E = 21.4
          #kcal/mol
R = 0.001987
          #kcal/mol.K

#RELATIVE RATE:
ra = -rw                        #mol/m3.s
rc = -rw
rl = rw

#STOICHIOMETRY (assume liquid phase or aqueous, project statement-stoichionmetric equivalents)
Ct = Ca+Cc+Cl+Cw                #mol/m3

xa = Ca/Ct
xc = Cc/Ct
xl = Cl/Ct
xw = Cw/Ct

Fa = Ca*vo
Fc = Cc*vo
Fw = Cw*vo
#Fl = Cl*vo

#ENERGY BALANCE (assume CSTR, with HEX:steam, or downtherm boiler)
f(T) =U*A*(Ta-T)-Fao*(Cpa+Cpc)*(T-To)+deltaH*ra*V
          # Energy balance, Fogler p.567
T(0) = 520
deltaH = deltaHo*4.184+(Cpl+Cpw-Cpa-Cpc)*(T-Tr)
          #J/mol
Cpa = 68.14
          #J/mol.K, calculated, literature, check "chemical property" Spreadsheet
Cpc = 275.37
Cpl = 377.92
Cpw = 75.4

#Q = Fl*Cpl*(T-To)
          #J/s=W
#UA = Q/(((Ta-T)-(Ta-To))/ln((Ta-T)/(Ta-To)))
          #J/s.K
#deltaTlm = ((Ts-T)-(Ts-To))/ln((Ts-T)/(Ts-To))
```

POLYMATH Report
Nonlinear Equations

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	Ca	462.8893	2.576E-14	1.0E-06
2	Cc	462.8893	2.665E-14	1.0E-05
3	Cl	5037.561	-2.487E-14	2000.
4	Cw	1.054E+04	-2.398E-14	10000.
5	T	541.1971	1.019E-09	520.

	Variable	Value
1	A	34.63136
2	Cao	5500.45
3	Cco	5500.45
4	Cpa	68.14
5	Cpc	275.37
6	Cpl	377.92
7	Cpw	75.4
8	Ct	1.65E+04
9	Cwo	5500.45
10	deltaH	2.487E+04
11	deltaHo	4153.798
12	E	21.4
13	Fa	0.5228404
14	Fao	6.21284
15	Fc	0.5228404
16	Fco	6.21284
17	Fl	5.69
18	Fw	11.90284
20	K	531.0598
21	k	145.4477
22	ko	8.2531
23	Ko	304.2805
24	p	0.9158452
25	R	0.001987
26	ra	-0.2798645
27	rc	-0.2798645
28	rl	0.2798645
29	rw	0.2798645
30	Ta	573.
31	tau	1.8E+04
32	To	463.
33	Tr	473.
34	U	280.
35	V	20.33127
36	vo	0.0011295
37	xa	0.0280516
38	xc	0.0280516
39	xl	0.3052817
40	xw	0.6386151

Figure A.1: Polymath Report for the Chemical Reaction Kinetics of the Polymerization CSTR with Full Capacity

Explicit equations

1 Fl = 5.69

mol/s, calculated, 0.95 service factor

2 tau = 18000

in sec, Ogata 5 hours residence time, Fogler: 10min-4hour for industrial CSTR

3 To = 190+273

Ogata, range 200-220C

4 Ta = 573

K, Dowtherm a, maximum 400 degree C, Turton heuristic

5 V = Fl*226.3/1140000*tau

m3

6 A = 2*3.14*((2*V/3.14)^(1/3))^2

m2, D=L, H=2L

7 U = 280

J/m2.s.K, Heuristic

8 vo = V/tau

m3/s

9 Ct = Ca+Cc+Cl+Cw

mol/m3

10 Fa = Ca*vo

11 E = 21.4

kcal/mol

12 Tr = 473

in K, Steppan

13 R = 0.001987

kcal/mol.K

14 xc = Cc/Ct

15 xl = Cl/Ct

16 xa = Ca/Ct

17 xw = Cw/Ct

18 ko = exp(2.55-0.45*tanh(25*(xw-0.55)))+8.58*(tanh(50*(xw-0.10))-1)*(1-30.05*xc)

ko[=]1/hr; ko,Ko and detaHo models from Steppan

19 Ko = exp((1-0.47*exp(-xw^(1/2)/0.2))*(8.45-4.2*xw))

20 k = ko *exp(E/R*(1/Tr-1/T))

1/hr, Arrhenius equation at a convenient Temp. Tr=200C

Figure A.1: Polymath Report for the Chemical Reaction Kinetics of the Polymerization CSTR with 100% Capacity (continued)

```
20 k = ko *exp(E/R*(1/Tr-1/T))
   1/hr, Arrhenius equation at a convenient Temp. Tr=200C
21 deltaHo = 7650*tanh(6.5*(xw-0.52))+6500*exp(-xw/0.065)-800
   cal/mol, convert to J/mol: multiply 4.184
22 K = Ko *exp(deltaHo*10^(-3)/R*(1/Tr-1/T))
   literature used: Steppan
23 rw = Ct*k/3600*(xa*xc-xl*xw/K)
   Steppan and Giudici, r in mol/m3.s
24 rl = rw
25 ra = -rw
   mol/m3.s
26 Fao = (0-Fl)/(-rl)*(-ra)+Fa
27 Cao = Fao/vo
   mol/m3
28 Fco = Fao
29 Fwo = Fao
   use molar ratio from Ogata: range 0.5-10 : salt/water
30 Cwo = Fwo/vo
31 rc = -rw
32 p = 1-Ca/Cao
   fraction of functional group amine (a), MIGHT be able to use for optimization,
33 Cco = Fao/vo
   assuming Fao=Fco, due to stoichiometric equivalence
34 Fc = Cc*vo
35 Fw = Cw*vo
36 Cpw = 75.4
37 Cpa = 68.14
   J/mol.K, calculated, literature, check "chemical property" Spreadsheet
38 Cpc = 275.37
39 Cpl = 377.92
40 deltaH = deltaHo*4.184+(Cpl+Cpw-Cpa-Cpc)*(T-Tr)
   J/mol
```

Figure A.1: Polymath Report for the Chemical Reaction Kinetics of the Polymerization CSTR with 100% Capacity (continued)

POLYMATH Report
Nonlinear Equations

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	Ca	419.613	6.217E-15	1.0E-06
2	Cc	419.613	6.217E-15	1.0E-05
3	Cl	5037.561	-6.661E-15	2000.
4	Cw	1.049E+04	-7.105E-15	10000.
5	T	550.0062	4.948E-10	520.

	Variable	Value
1	A	34.62
2	Cao	5457.174
3	Cco	5457.174
4	Cpa	68.14
5	Cpc	275.37
6	Cpl	377.92
7	Cpw	75.4
8	Ct	1.637E+04
9	Cwo	5457.174
10	deltaH	2.613E+04
11	deltaHo	4222.984
12	E	21.4
13	Fa	0.317361
14	Fao	4.127361
15	Fc	0.317361
16	Fco	4.127361
17	Fl	3.81
18	Fw	7.937361
20	K	565.2925
21	k	199.8074
22	ko	8.243247
23	Ko	301.3418
24	p	0.923108
25	R	0.001987
26	ra	-0.2798645
27	rc	-0.2798645
28	rl	0.2798645
29	rw	0.2798645
30	Ta	573.
31	tau	1.8E+04
32	To	463.
33	Tr	473.
34	U	280.
35	V	13.61373
36	vo	0.0007563
37	xa	0.0256307
38	xc	0.0256307
39	xl	0.3077027
40	xw	0.641036

Figure A.2: Polymath Report for the Chemical Reaction Kinetics of the Polymerization CSTR with 67% Capacity

Polymath Coding of the Chemical Reaction Engineering Algorithm Modeling Using Polymath for Autoclave (Polymerization reactor) as a CSTR at STARTUP

```
#Components: a-amine end-group, c-carbonxyl end-group, l-amide linkage (nylon 6,6), w-water molecule

#DESIGN SPECIFICATION AND INITIAL CONDITION
#Ml =85E6                                   #lbm/year
#MWl = 226.3                                #g/mol, polymer data handbook
#densityl = 1140000                         #g/m3
Fl = 5.69                                   #mol/s, calculated, 0.95 service factor
#ml = 1286.93                               #g/s
tau = 18000                                 #in sec, Ogata 5 hours residence time,
Fogler: 10min-4hour for industrial CSTR
To = 190+273                                #Ogata, range 200-220C
Ta = 573                                    #K, Dowtherm a, maximum 400 degree
C, Turton heuristic
#T = 520                                    #K
#Ts = 550
V = Fl*226.3/1140000*tau                    #m3
A = 2*3.14*((2*V/3.14)^(1/3))^2             #m2, D=L, H=2L
U = 280                                     #J/m2.s.K, Heuristic
vo = V/tau                                  #m3/s
p = 1-Ca/Cao                                # fraction of functional group amine (a),
MIGHT be able to use for optimization,

#Fao = Fa/(1-p)
Fao = (0-Fl)/(-rl)*(-ra)+Fa
Fco = Fao
Fwo = Fao                                   #use molar ratio from Ogata: range 0.5-
10 : salt/water

#Flo = 0
Cao = Fao/vo                                #mol/m3
Cco = Fao/vo                                #assuming Fao=Fco, due to
stoichiometric equivalence
Cwo = Fwo/vo


#MOLE BALANCE (single reaction, single phase, reversible, CSTR)
f(Ca) = vo*Cao-vo*Ca+ra*V
Ca(0) = 0.000001
f(Cc) = vo*Cco-vo*Cc+rc*V
Cc(0) =0.00001
f(Cl) = -vo*Cl+rl*V
Cl(0) = 2000
f(Cw) = vo*Cwo-vo*Cw+rw*V
Cw(0) = 10000

#RATE LAW (activate if reversible, homogeneous rxn)
rw = Ct*k/3600*(xa*xc-xl*xw/K)
        #Steppan and Giudici, r in mol/m3.s

        #rw is positive due to water being product

k = ko *exp(E/R*(1/Tr-1/T))
        #1/hr, Arrhenius equation at a convenient Temp. Tr=200C
```

Polymath Coding of the Chemical Reaction Engineering Algorithm Modeling Using Polymath for Autoclave (Polymerization reactor) as a CSTR at STARTUP (continued)

```
K = Ko *exp(deltaHo*10^(-3)/R*(1/Tr-1/T))
                    #literature used: Steppan

ko = exp(2.55-0.45*tanh(25*(xw-0.55)))+8.58*(tanh(50*(xw-0.10))-1)*(1-30.05*xc)
          #ko[=]1/hr; ko,Ko and detaHo models from Steppan
Ko = exp((1-0.47*exp(-xw^(1/2)/0.2))*(8.45-4.2*xw))
deltaHo = 7650*tanh(6.5*(xw-0.52))+6500*exp(-xw/0.065)-800
          #cal/mol, convert to J/mol: multiply 4.184

Tr = 473
          #in K, Steppan
E = 21.4
          #kcal/mol
R = 0.001987
          #kcal/mol.K

#RELATIVE RATE:
ra = -rw                              #mol/m3.s
rc = -rw
rl = rw

#STOICHIOMETRY (assume liquid phase or aqueous, project statement-stoichionmetric equivalents)
Ct = Ca+Cc+Cl+Cw                      #mol/m3

xa = Ca/Ct
xc = Cc/Ct
xl = Cl/Ct
xw = Cw/Ct

Fa = Ca*vo
Fc = Cc*vo
Fw = Cw*vo
#Fl = Cl*vo

#ENERGY BALANCE (assume CSTR, with HEX:steam, or downtherm boiler)
f(T) =U*A*(Ta-T)-Fao*(Cpa+Cpc)*(T-To)+deltaH*ra*V
          # Energy balance, Fogler p.567
T(0) = 520

deltaH = deltaHo*4.184+(Cpl+Cpw-Cpa-Cpc)*(T-Tr)
          #J/mol
Cpa = 68.14
          #J/mol.K, calculated, literature, check "chemical property" Spreadsheet
Cpc = 275.37
Cpl = 377.92
Cpw = 75.4

#Q = Fl*Cpl*(T-To)
          #J/s=W
#UA = Q/(((Ta-T)-(Ta-To))/ln((Ta-T)/(Ta-To)))

          #J/s.K
#deltaTlm = ((Ts-T)-(Ts-To))/ln((Ts-T)/(Ts-To))
```

POLYMATH Report
Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	A	26.4882	26.4882	26.4882	26.4882
2	Ca	5457.174	401.2101	5457.174	401.2101
3	Cao	5457.174	5457.174	5457.174	5457.174
4	Cc	5457.174	401.2101	5457.174	401.2101
5	Cco	5457.174	5457.174	5457.174	5457.174
6	Cl	0.0001	0.0001	5055.964	5055.964
7	Cpa	68.14	68.14	68.14	68.14
8	Cpc	275.37	275.37	275.37	275.37
9	Cpl	377.92	377.92	377.92	377.92
10	Cpw	75.4	75.4	75.4	75.4
11	Ct	1.637E+04	1.637E+04	1.637E+04	1.637E+04
12	Cw	5457.174	5457.174	1.051E+04	1.051E+04
13	Cwo	5457.174	5457.174	5457.174	5457.174
14	deltaH	-4.318E+04	-4.318E+04	2.681E+04	2.681E+04
15	deltaHo	-7169.699	-7169.699	4254.626	4254.626
16	E	21.4	21.4	21.4	21.4
17	Fa	4.123198	0.3031365	4.123198	0.3031365
18	Fao	4.123198	4.123198	4.123198	4.123198
19	Fc	4.123198	0.3031365	4.123198	0.3031365
20	Fco	4.123198	4.123198	4.123198	4.123198
21	Fl	7.556E-08	7.556E-08	3.820062	3.820062
22	Fw	4.123198	4.123198	7.94326	7.94326
23	Fwo	4.123198	4.123198	4.123198	4.123198

Figure A.3: Polymath Report for the Chemical Reaction Kinetics of the Polymerization CSTR at Startup

23	Fwo	4.123198	4.123198	4.123198	4.123198
24	k	0.0087353	0.0087353	238.3376	238.3376
25	K	1.282E+04	420.8026	1.282E+04	585.6417
26	Ko	958.3845	299.9865	958.3845	299.9865
27	ko	20.08518	8.239057	20.08518	8.239057
28	p	1.832E-08	1.832E-08	0.9264802	0.9264802
29	R	0.001987	0.001987	0.001987	0.001987
30	ra	-0.0044139	-3.401308	-0.0044139	-0.2839123
31	rc	-0.0044139	-3.401308	-0.0044139	-0.2839123
32	rl	0.0044139	0.0044139	3.401308	0.2839123
33	rw	0.0044139	0.0044139	3.401308	0.2839123
34	T	353.	353.	555.0186	555.0186
35	t	0	0	1.8E+04	1.8E+04
36	Ta	573.	573.	573.	573.
37	tau	1.8E+04	1.8E+04	1.8E+04	1.8E+04
38	To	463.	463.	463.	463.
39	Tr	473.	473.	473.	473.
40	U	280.	280.	280.	280.
41	V	13.6	13.6	13.6	13.6
42	vo	0.0007556	0.0007556	0.0007556	0.0007556
43	xa	0.3333333	0.0245066	0.3333333	0.0245066
44	xc	0.3333333	0.0245066	0.3333333	0.0245066
45	xl	6.108E-09	6.108E-09	0.3088268	0.3088268
46	xw	0.3333333	0.3333333	0.6421601	0.6421601

Differential equations

1 d(Ca)/d(t) = ra + (Cao-Ca)*vo/V

2 d(Cc)/d(t) = rc + (Cco-Cc)*vo/V

3 d(Cl)/d(t) = rl+(-Cl)*vo/V

4 d(Cw)/d(t) = rw + (Cwo-Cw)*vo/V

5 d(T)/d(t) = (ra*V*deltaH-U*A*(T-Ta))/(V*(Ca*Cpa+Cc*Cpc+Cl*Cpl+Cw*Cpw))

Figure A.3: Polymath Report for the Chemical Reaction Kinetics of the Polymerization CSTR at STARTUP (continued)

Explicit equations

1 V = 13.6

m3, Check "Ye Notebook"

2 tau = 18000

in sec, Ogata 5 hours residence time, Fogler: 10min-4hour for industrial CSTR

3 To = 190+273

Ogata, range 200-220C

4 Ta = 573

K, dependent on steam using, high pressure

5 vo = V/tau

m3/s

6 E = 21.4

kcal/mol

7 U = 280

8 A = 2*3.14*((2*V/3.14)^(1/3))^2

m2, D=L, H=2L

9 FI = CI*vo

10 Tr = 473

in K, Steppan

11 Ct = Ca+Cc+CI+Cw

mol/m3

12 xa = Ca/Ct

13 Fa = Ca*vo

mol/s

14 R = 0.001987

kcal/mol.K

15 xI = CI/Ct

16 xw = Cw/Ct

17 xc = Cc/Ct

18 Ko = exp((1-0.47*exp(-xw^(1/2)/0.2))*(8.45-4.2*xw))

19 ko = exp(2.55-0.45*tanh(25*(xw-0.55)))+8.58*(tanh(50*(xw-0.10))-1)*(1-30.05*xc)

ko[=]1/hr; ko,Ko and detaHo models from Steppan

Figure A.3: Polymath Report for the Chemical Reaction Kinetics of the Polymerization CSTR at Startup (continued)

```
19 ko = exp(2.55-0.45*tanh(25*(xw-0.55)))+8.58*(tanh(50*(xw-0.10))-1)*(1-30.05*xc)
   ko[=]1/hr; ko,Ko and detaHo models from Steppan
20 deltaHo = 7650*tanh(6.5*(xw-0.52))+6500*exp(-xw/0.065)-800
   cal/mol, convert to J/mol: multiply 4.184
21 K = Ko *exp(deltaHo*10^(-3)/R*(1/Tr-1/T))
   literature used: Steppan
22 k = ko *exp(E/R*(1/Tr-1/T))
   1/hr, Arrhenius equation at a convenient Temp. Tr=200C
23 rw = Ct*k/3600*(xa*xc-xl*xw/K)
   Steppan and Giudici, r in mol/m3.s
24 ra = -rw
   mol/m3.s
25 rl = rw
26 Fao = (0-Fl)/(-rl)*(-ra)+Fa
27 Cao = Fao/vo
   mol/m3
28 Fco = Fao
29 Fwo = Fao
30 rc = -rw
31 Cwo = Fwo/vo
32 p = 1-Ca/Cao
   fraction of functional group amine (a), MIGHT be able to use for optimization,
33 Fc = Cc*vo
34 Fw = Cw*vo
35 Cco = Fao/vo
   assuming Fao=Fco, due to stoichiometric equivalence
36 Cpw = 75.4
37 Cpa = 68.14
   J/mol.K, calculated, literature, check "chemical property" Spreadsheet
38 Cpc = 275.37
39 Cpl = 377.92
40 deltaH = deltaHo*4.184+(Cpl+Cpw-Cpa-Cpc)*(T-Tr)
   J/mol
```

Figure A.3: Polymath Report for the Chemical Reaction Kinetics of the Polymerization CSTR at Startup (continued)

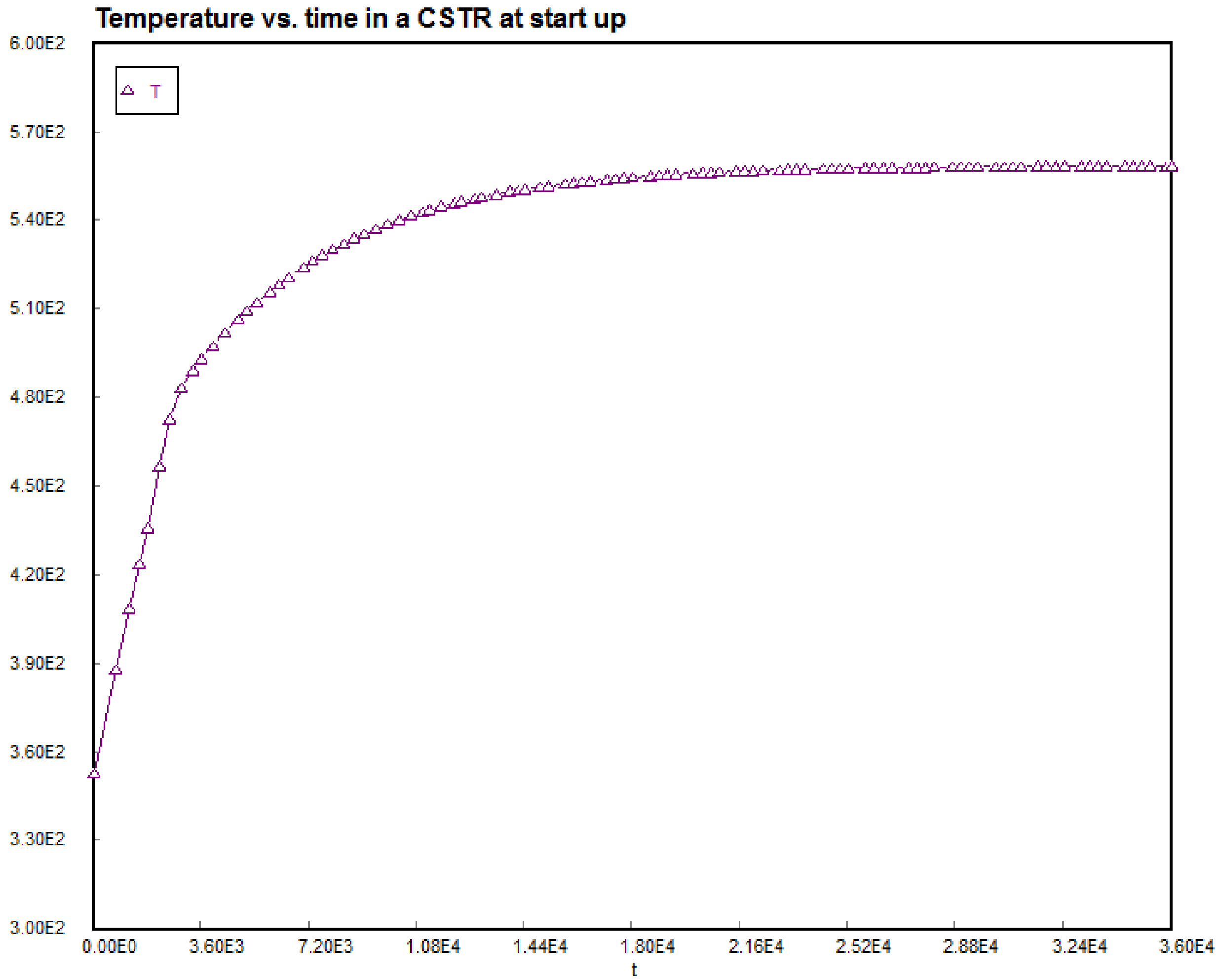

Figure A.4: Polymath Plot of the Reaction Temperature vs. Time for the Polymerization CSTR at Startup

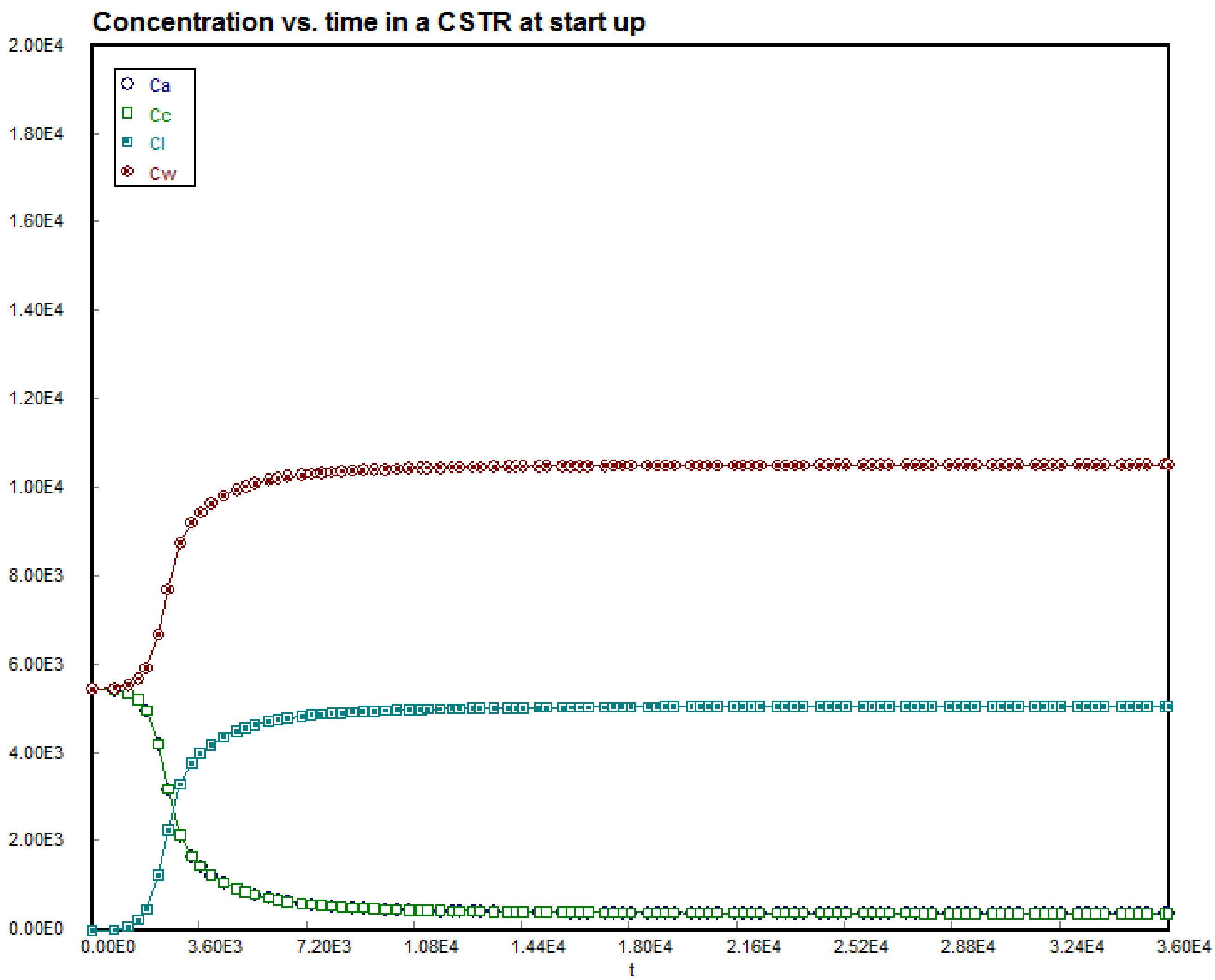

Figure A.5: Polymath Plot of the Components Concentration vs. Time for the Polymerization CSTR at Startup

Safety Data Sheets:

SIGMA-ALDRICH

sigma-aldrich.com

SAFETY DATA SHEET

Version 5.9
Revision Date 05/23/2016
Print Date 01/23/2017

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name	:	Hexamethylenediamine
Product Number	:	H11696
Brand	:	Aldrich
Index-No.	:	612-104-00-9
CAS-No.	:	124-09-4

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company	:	Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	:	+1 800-325-5832
Fax	:	+1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Dermal (Category 4), H312
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Acute aquatic toxicity (Category 3), H402

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word: Danger

Hazard statement(s)

H302 + H312	Harmful if swallowed or in contact with skin
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H335	May cause respiratory irritation.
H402	Harmful to aquatic life.

Precautionary statement(s)

P260	Do not breathe dust or mist.

Aldrich - H11696 Page 1 of 8

Figure A.6: Safety Data Sheet for HMDA [4]

P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/doctor.
P363	Wash contaminated clothing before reuse.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	1,6-Diaminohexane 1,6-Hexanediamine
Formula	:	$C_6H_{16}N_2$
Molecular weight	:	116.20 g/mol
CAS-No.	:	124-09-4
EC-No.	:	204-679-6
Index-No.	:	612-104-00-9

Hazardous components

Component	Classification	Concentration
Hexamethylenediamine		
	Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; STOT SE 3; Aquatic Acute 3; H302 + H312, H314, H318, H335, H402	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.Continue rinsing eyes during transport to hospital.

Figure A.6: Safety Data Sheet for HMDA [4]

Component	CAS-No.	Value	Control parameters	Basis
Hexamethylenediamine	124-09-4	TWA	0.500000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Skin irritation		
		TWA	1.000000 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
		PEL	0.5 ppm 2.3 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 480 min
Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 60 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance Form: solid

Aldrich - H11696 Page 4 of 8

Aldrich - H11696 Page 3 of 8

Figure A.6: Safety Data Sheet for HMDA [4]

		Colour: colourless
b)	Odour	No data available
c)	Odour Threshold	No data available
d)	pH	12.4 at 100 g/l at 25 °C (77 °F)
e)	Melting point/freezing point	Melting point/range: 42 - 45 °C (108 - 113 °F) - lit.
f)	Initial boiling point and boiling range	204 - 205 °C (399 - 401 °F)
g)	Flash point	80 °C (176 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 6.3 %(V) Lower explosion limit: 0.7 %(V)
k)	Vapour pressure	No data available
l)	Vapour density	4.01 - (Air = 1.0)
m)	Relative density	0.89 g/cm3 at 25 °C (77 °F)
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	log Pow: 0.02
p)	Auto-ignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

Relative vapour density 4.01 - (Air = 1.0)

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
hygroscopic
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
No data available

10.5 Incompatible materials
acids, Acid chlorides, Acid anhydrides, Strong oxidizing agents, Carbon dioxide (CO2)

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)
Other decomposition products - No data available
In the event of fire: see section 5

Figure A.6: Safety Data Sheet for HMDA [4]

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 750 mg/kg

LD50 Dermal - Rabbit - 1,110 mg/kg

No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitisation
No data available

Germ cell mutagenicity
No data available

Carcinogenicity

IARC:	No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP:	No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA:	No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
No data available

No data available

Specific target organ toxicity - single exposure
May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Additional Information
RTECS: MO1180000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Liver - Irregularities - Based on Human Evidence
Liver - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	LC50 - Leuciscus idus (Golden orfe) - 62 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 23.4 mg/l - 48 h

12.2 Persistence and degradability
No data available

Figure A.6: Safety Data Sheet for HMDA [4]

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 2280 Class: 8 Packing group: III
Proper shipping name: Hexamethylenediamine, solid
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG
UN number: 2280 Class: 8 Packing group: III EMS-No: F-A, S-B
Proper shipping name: HEXAMETHYLENEDIAMINE, SOLID

IATA
UN number: 2280 Class: 8 Packing group: III
Proper shipping name: Hexamethylenediamine, solid

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Hexamethylenediamine	124-09-4	1993-04-24

	CAS-No.	Revision Date
Hexamethylenediamine	124-09-4	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Hexamethylenediamine	124-09-4	1993-04-24

Figure A.6: Safety Data Sheet for HMDA [4]

	CAS-No.	Revision Date
Hexamethylenediamine	124-09-4	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
Hexamethylenediamine	124-09-4	1993-04-24

	CAS-No.	Revision Date
Hexamethylenediamine	124-09-4	1993-04-24

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Eye Dam.	Serious eye damage
H302	Harmful if swallowed.
H302 + H312	Harmful if swallowed or in contact with skin
H312	Harmful in contact with skin.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H335	May cause respiratory irritation.

HMIS Rating

Health hazard:	3
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	0

NFPA Rating

Health hazard:	3
Fire Hazard:	2
Reactivity Hazard:	0

Further information

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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.9 Revision Date: 05/23/2016 Print Date: 01/23/2017

Figure A.6: Safety Data Sheet for HMDA [4]

Adipic Acid

SIGMA-ALDRICH

sigma-aldrich.com

SAFETY DATA SHEET

Version 4.11
Revision Date 05/06/2016
Print Date 01/23/2017

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Adipic acid

Product Number : A26357
Brand : Sigma
Index-No. : 607-144-00-9

CAS-No. : 124-04-9

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Eye irritation (Category 2A), H319
Acute aquatic toxicity (Category 3), H402

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word: Warning

Hazard statement(s)

H319	Causes serious eye irritation.
H402	Harmful to aquatic life.

Precautionary statement(s)

P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear eye protection/ face protection.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P501	Dispose of contents/ container to an approved waste disposal plant.

Sigma - A26357 Page 1 of 8

Figure A.7: Safety Data Sheet for Adipic Acid [5]

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Combustible dust

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	Hexanedioic acid ADI-PURE® high purity adipic acid ADI-PURE® LGA adipic acid
Formula	:	$C_6H_{10}O_4$
Molecular weight	:	146.14 g/mol
CAS-No.	:	124-04-9
EC-No.	:	204-673-3
Index-No.	:	607-144-00-9

Hazardous components

Component	Classification	Concentration
Adipic acid		
	Eye Irrit. 2A; Aquatic Acute 3; H319, H402	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

Figure A.7: Safety Data Sheet for Adipic Acid [5]

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.Avoid contact with skin and eyes. Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Adipic acid	124-04-9	TWA	5.000000 mg/m3	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation ANS impairment		
		TWA	5 mg/m3	USA. ACGIH Threshold Limit Values (TLV)
		Upper Respiratory Tract irritation ANS impairment		
		PEL	5 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Figure A.7: Safety Data Sheet for Adipic Acid [5]

m)	Relative density	No data available
n)	Water solubility	23 g/l at 25 °C (77 °F) - soluble
o)	Partition coefficient: n-octanol/water	log Pow: 0.093 at 25 °C (77 °F)
p)	Auto-ignition temperature	> 400 °C (> 752 °F)
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	Not explosive
t)	Oxidizing properties	No data available

9.2 Other safety information

Bulk density	0.7 g/l
Solubility in other solvents	Methanol - soluble Ethanol - soluble Acetone - soluble Benzene - slightly soluble
Dissociation constant	4.43 at 20 °C (68 °F)

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
No data available

10.5 Incompatible materials
Strong oxidizing agents

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 5,560 mg/kg
(OECD Test Guideline 401)

LC0 Inhalation - Rat - male and female - 4 h - > 7.7 mg/l
(OECD Test Guideline 403)

LD0 Dermal - Rabbit - male and female - 7,940 mg/kg

No data available

Skin corrosion/irritation
No data available

Figure A.7: Safety Data Sheet for Adipic acid [5]

Serious eye damage/eye irritation
Respiratory or skin sensitisation
Maximisation Test - Guinea pig
Result: Does not cause skin sensitisation.

Germ cell mutagenicity
Hamster
fibroblast
Result: negative

Rat - male
Result: negative

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
No data available

No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Additional Information
RTECS: AU8400000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	static test LC0 - Brachydanio rerio (zebrafish) - >= 1,000 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates	Immobilization LC50 - Daphnia magna (Water flea) - 46 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test EC50 - Pseudokirchneriella subcapitata (algae) - 59 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	Respiration inhibition EC50 - Sludge Treatment - 7,910 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 30 d Result: 83 % - Readily biodegradable (OECD Test Guideline 301D)

12.3 Bioaccumulative potential
No data available

Figure A.7: Safety Data Sheet for Adipic acid [5]

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Eye Irrit.	Eye irritation
H319	Causes serious eye irritation.
H402	Harmful to aquatic life.

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	1
Reactivity Hazard:	0

Further information

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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 4.11 Revision Date: 06/06/2016 Print Date: 01/23/2017

Adipic acid 124-04-9 1993-04-24

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

Figure A.7: Safety Data Sheet for Adipic Acid [5]

Nylon 6 6

SIGMA-ALDRICH

sigma-aldrich.com

SAFETY DATA SHEET

Version 4.2
Revision Date 06/30/2014
Print Date 01/23/2017

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name	:	Nylon 6/6
Product Number	:	429171
Brand	:	Aldrich
CAS-No.	:	32131-17-2

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses	:	Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company	:	Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	:	+1 800-325-5832
Fax	:	+1 800-325-5052

1.4 Emergency telephone number

Emergency Phone #	:	+1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

Not a hazardous substance or mixture.

2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	Poly(N,N'-hexamethyleneadipinediamide Poly(hexamethylene adipamide)
Formula	:	$C_{12}H_{26}N_2O_4$
Molecular Weight	:	262.35 g/mol
CAS-No.	:	32131-17-2

No ingredients are hazardous according to OSHA criteria.
No components need to be disclosed according to the applicable regulations.

4. FIRST AID MEASURES

4.1 Description of first aid measures

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration.

Aldrich - 429171 Page 1 of 6

Figure A.8: Safety Data Sheet for Nylon 6 6 [48]

In case of skin contact
Wash off with soap and plenty of water.

In case of eye contact
Flush eyes with water as a precaution.

If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
no data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides, nitrogen oxides (NOx)

5.3 Advice for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information
no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Avoid dust formation. Avoid breathing vapours, mist or gas.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Provide appropriate exhaust ventilation at places where dust is formed.Normal measures for preventive fire protection.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
General industrial hygiene practice.

Aldrich - 429171 Page 2 of 6

Figure A.8: Safety Data Sheet for Nylon 6 6 [48]

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection
Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: pellets Colour: white
b)	Odour	no data available
c)	Odour Threshold	no data available
d)	pH	no data available
e)	Melting point/freezing point	Melting point/range: 250 - 260 °C (482 - 500 °F) - lit.
f)	Initial boiling point and boiling range	no data available
g)	Flash point	no data available
h)	Evapouration rate	no data available
i)	Flammability (solid, gas)	no data available
j)	Upper/lower flammability or explosive limits	no data available
k)	Vapour pressure	no data available
l)	Vapour density	no data available
m)	Relative density	1.14 g/mL at 25 °C (77 °F)
n)	Water solubility	no data available
o)	Partition coefficient: n-octanol/water	no data available
p)	Auto-ignition temperature	no data available
q)	Decomposition temperature	no data available
r)	Viscosity	no data available
s)	Explosive properties	no data available

Figure A.8: Safety Data Sheet for Nylon 6 6 [48]

t) Oxidizing properties no data available

9.2 Other safety information
no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
no data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
no data available

10.4 Conditions to avoid
no data available

10.5 Incompatible materials
Strong oxidizing agents, Strong bases

10.6 Hazardous decomposition products
Other decomposition products - no data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
no data available

Inhalation: no data available

Dermal: no data available

no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitisation
no data available

Germ cell mutagenicity
no data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
no data available

no data available

Specific target organ toxicity - single exposure
no data available

Aldrich - 429171 Page 4 of 6

Figure A.8: Safety Data Sheet for Nylon 6 6 [48]

Specific target organ toxicity - repeated exposure
no data available

Aspiration hazard
no data available

Additional Information
RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity
no data available

12.2 Persistence and degradability
no data available

12.3 Bioaccumulative potential
no data available

12.4 Mobility in soil
no data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
No SARA Hazards

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

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Figure A.8: Safety Data Sheet for Nylon 6 6 [48]

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Poly(N,N'-hexamethyleneadipinediamide	32131-17-2	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Poly(N,N'-hexamethyleneadipinediamide	32131-17-2	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

HMIS Rating

Health hazard:	0
Chronic Health Hazard:	
Flammability:	0
Physical Hazard	0

NFPA Rating

Health hazard:	0
Fire Hazard:	0
Reactivity Hazard:	0

Further information

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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 4.2 Revision Date: 06/30/2014 Print Date: 01/23/2017

Figure A.8: Safety Data Sheet for Nylon 6 6 [48]

Nitrogen

SAFETY DATA SHEET

Nitrogen

Airgas
an Air Liquide company

Section 1. Identification

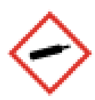
GHS product identifier	: Nitrogen
Chemical name	: nitrogen
Other means of identification	: nitrogen (dot); nitrogen gas; Nitrogen NF, Nitrogen FG
Product use	: Synthetic/Analytical chemistry.
Synonym	: nitrogen (dot); nitrogen gas; Nitrogen NF, Nitrogen FG
SDS #	: 001040
Supplier's details	: Airgas USA, LLC and its affiliates 259 North Radnor-Chester Road Suite 100 Radnor, PA 19087-5283 1-610-687-5253
24-hour telephone	: 1-866-734-3438

Section 2. Hazards identification

OSHA/HCS status	: This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
Classification of the substance or mixture	: GASES UNDER PRESSURE - Compressed gas

GHS label elements

Hazard pictograms :



Signal word	: Warning
Hazard statements	: Contains gas under pressure; may explode if heated. May displace oxygen and cause rapid suffocation.

Precautionary statements

General	: Read and follow all Safety Data Sheets (SDS'S) before use. Read label before use. Keep out of reach of children. If medical advice is needed, have product container or label at hand. Close valve after each use and when empty. Use equipment rated for cylinder pressure. Do not open valve until connected to equipment prepared for use. Use a back flow preventative device in the piping. Use only equipment of compatible materials of construction.
Prevention	: Not applicable.
Response	: Not applicable.
Storage	: Protect from sunlight when ambient temperature exceeds 52°C/125°F. Store in a well-ventilated place.
Disposal	: Not applicable.
Hazards not otherwise classified	: In addition to any other important health or physical hazards, this product may displace oxygen and cause rapid suffocation.

Date of issue/Date of revision : 5/26/2015 Date of previous issue : 8/7/2015 Version : 0.02 1/10

Figure A.9: Safety Data Sheet for Nitrogen [49]

Nitrogen

Section 3. Composition/information on ingredients

Substance/mixture : Substance

Chemical name : nitrogen

Other means of identification : nitrogen (dot); nitrogen gas; Nitrogen NF, Nitrogen FG

CAS number/other identifiers

CAS number : 7727-37-9

Product code : 001040

Ingredient name	%	CAS number
Nitrogen	100	7727-37-9

Any concentration shown as a range is to protect confidentiality or is due to batch variation.

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment and hence require reporting in this section.

Occupational exposure limits, if available, are listed in Section 8.

Section 4. First aid measures

Description of necessary first aid measures

Eye contact : Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention if irritation occurs.

Inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.

Skin contact : Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if symptoms occur. Wash clothing before reuse. Clean shoes thoroughly before reuse.

Ingestion : As this product is a gas, refer to the inhalation section.

Most important symptoms/effects, acute and delayed

Potential acute health effects

Eye contact : Contact with rapidly expanding gas may cause burns or frostbite.

Inhalation : No known significant effects or critical hazards.

Skin contact : Contact with rapidly expanding gas may cause burns or frostbite.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Ingestion : As this product is a gas, refer to the inhalation section.

Over-exposure signs/symptoms

Eye contact : No specific data.

Inhalation : No specific data.

Skin contact : No specific data.

Ingestion : No specific data.

Indication of immediate medical attention and special treatment needed, if necessary

Notes to physician : In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.

Date of issue/Date of revision : 5/25/2015 *Date of previous issue* : 8/7/2015 *Version* : 0.02 2/10

Figure A.9: Safety Data Sheet for Nitrogen [49]

Nitrogen

Section 4. First aid measures

Specific treatments	: No specific treatment.
Protection of first-aiders	: No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

See toxicological information (Section 11)

Section 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media	: Use an extinguishing agent suitable for the surrounding fire.
Unsuitable extinguishing media	: None known.
Specific hazards arising from the chemical	: Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.
Hazardous thermal decomposition products	: Decomposition products may include the following materials: nitrogen oxides
Special protective actions for fire-fighters	: Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Contact supplier immediately for specialist advice. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.
Special protective equipment for fire-fighters	: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

For non-emergency personnel	: No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Avoid breathing gas. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
For emergency responders	: If specialised clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".
Environmental precautions	: Ensure emergency procedures to deal with accidental gas releases are in place to avoid contamination of the environment. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Methods and materials for containment and cleaning up

Small spill	: Immediately contact emergency personnel. Stop leak if without risk.
Large spill	: Immediately contact emergency personnel. Stop leak if without risk. Note: see Section 1 for emergency contact information and Section 13 for waste disposal.

Section 7. Handling and storage

Precautions for safe handling

Protective measures	: Put on appropriate personal protective equipment (see Section 8). Contains gas under pressure. Avoid contact with eyes, skin and clothing. Avoid breathing gas. Empty containers retain product residue and can be hazardous. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Date of issue/Date of revision : 5/25/2015 *Date of previous issue* : 8/7/2015 *Version* : 0.02 3/10

Figure A.9: Safety Data Sheet for Nitrogen [49]

Nitrogen

Section 7. Handling and storage

Advice on general occupational hygiene : Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

Conditions for safe storage, including any incompatibilities : Store in accordance with local regulations. Store in a segregated and approved area. Store away from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10). Keep container tightly closed and sealed until ready for use. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Control parameters

Occupational exposure limits

Ingredient name	Exposure limits
Nitrogen	Oxygen Depletion [Asphyxiant]

Appropriate engineering controls : Good general ventilation should be sufficient to control worker exposure to airborne contaminants.

Environmental exposure controls : Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

Individual protection measures

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Eye/face protection : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: safety glasses with side-shields.

Skin protection

Hand protection : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.

Body protection : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Other skin protection : Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory protection : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

Date of issue/Date of revision : 5/25/2015 *Date of previous issue* : 8/7/2015 *Version* : 0.02 4/10

Figure A.9: Safety Data Sheet for Nitrogen [49]

Nitrogen

Section 9. Physical and chemical properties

Appearance	
Physical state	: Gas. [Compressed gas.]
Color	: Colorless.
Molecular weight	: 28.02 g/mole
Molecular formula	: N2
Boiling/condensation point	: -196°C (-320.8°F)
Melting/freezing point	: -210.01°C (-346°F)
Critical temperature	: -146.95°C (-232.5°F)
Odor	: Odorless.
Odor threshold	: Not available.
pH	: Not available.
Flash point	: [Product does not sustain combustion.]
Burning time	: Not applicable.
Burning rate	: Not applicable.
Evaporation rate	: Not available.
Flammability (solid, gas)	: Not available.
Lower and upper explosive (flammable) limits	: Not available.
Vapor pressure	: Not available.
Vapor density	: 0.967 (Air = 1) Liquid Density@BP: 50.46 lb/ft3 (808.3 kg/m3)
Specific Volume (ft ^{3}/lb)	: 13.8889
Gas Density (lb/ft ^{3})	: 0.072
Relative density	: Not applicable.
Solubility	: Not available.
Solubility in water	: Not available.
Partition coefficient: n-octanol/water	: 0.67
Auto-ignition temperature	: Not available.
Decomposition temperature	: Not available.
SADT	: Not available.
Viscosity	: Not applicable.

Section 10. Stability and reactivity

Reactivity	: No specific test data related to reactivity available for this product or its ingredients.
Chemical stability	: The product is stable.
Possibility of hazardous reactions	: Under normal conditions of storage and use, hazardous reactions will not occur.
Conditions to avoid	: No specific data.
Incompatible materials	: No specific data.
Hazardous decomposition products	: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization	: Under normal conditions of storage and use, hazardous polymerization will not occur.

Date of issue/Date of revision : 5/25/2015 *Date of previous issue* : 8/7/2015 *Version* : 0.02 5/10

Figure A.9: Safety Data Sheet for Nitrogen [49]

Nitrogen

Section 10. Stability and reactivity

Irritation/Corrosion

Not available.

Sensitization

Not available.

Mutagenicity

Not available.

Carcinogenicity

Not available.

Reproductive toxicity

Not available.

Teratogenicity

Not available.

Specific target organ toxicity (single exposure)

Not available.

Specific target organ toxicity (repeated exposure)

Not available.

Aspiration hazard

Not available.

Information on the likely routes of exposure : Not available.

Potential acute health effects

Eye contact	: Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation	: No known significant effects or critical hazards.
Skin contact	: Contact with rapidly expanding gas may cause burns or frostbite.
Ingestion	: As this product is a gas, refer to the inhalation section.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact	: No specific data.
Inhalation	: No specific data.
Skin contact	: No specific data.
Ingestion	: No specific data.

Delayed and immediate effects and also chronic effects from short and long term exposure

Short term exposure

Potential immediate effects	: Not available.
Potential delayed effects	: Not available.

Long term exposure

Potential immediate effects	: Not available.
Potential delayed effects	: Not available.

Potential chronic health effects

Not available.

General	: No known significant effects or critical hazards.
Carcinogenicity	: No known significant effects or critical hazards.

Date of issue/Date of revision : 5/25/2016 Date of previous issue : 8/7/2015 Version : 0.02 5/10

Figure A.9: Safety Data Sheet for Nitrogen [49]

Section 11. Toxicological information

Mutagenicity : No known significant effects or critical hazards.
Teratogenicity : No known significant effects or critical hazards.
Developmental effects : No known significant effects or critical hazards.
Fertility effects : No known significant effects or critical hazards.

Numerical measures of toxicity
Acute toxicity estimates
Not available.

Section 12. Ecological information

Toxicity
Not available.

Persistence and degradability
Not available.

Bioaccumulative potential

Product/ingredient name	$LogP_{ow}$	BCF	Potential
Nitrogen	0.67	-	low

Mobility in soil
Soil/water partition coefficient (K_{oc}) : Not available.

Other adverse effects : No known significant effects or critical hazards.

Section 13. Disposal considerations

Disposal methods : The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Empty Airgas-owned pressure vessels should be returned to Airgas. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. This material and its container must be disposed of in a safe way. Empty containers or liners may retain some product residues. Do not puncture or incinerate container.

Section 14. Transport information

	DOT	TDG	Mexico	IMDG	IATA
UN number	UN1066	UN1066	UN1066	UN1066	UN1066
UN proper shipping name	NITROGEN, COMPRESSED	NITROGEN, COMPRESSED	NITROGEN, COMPRESSED	NITROGEN, COMPRESSED	NITROGEN, COMPRESSED
Transport hazard class(es)	2.2	2.2	2.2	2.2	2.2

Figure A.9: Safety Data Sheet for Nitrogen [49]

Section 14. Transport information

Packing group	-	-	-	-	-
Environment	No.	No.	No.	No.	No.
Additional information	Limited quantity Yes. Packaging instruction Passenger aircraft Quantity limitation: 75 kg Cargo aircraft Quantity limitation: 150 kg	Product classified as per the following sections of the Transportation of Dangerous Goods Regulations: 2.13-2.17 (Class 2). Explosive Limit and Limited Quantity Index 0.125 Passenger Carrying Road or Rail Index 75	-	-	Passenger and Cargo Aircraft Quantity limitation: 75 kg Cargo Aircraft Only Quantity limitation: 150 kg

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Special precautions for user : **Transport within user's premises:** always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code : Not available.

Section 15. Regulatory information

U.S. Federal regulations : **TSCA 8(a) CDR Exempt/Partial exemption:** This material is listed or exempted.
United States inventory (TSCA 8b): This material is listed or exempted.

Clean Air Act Section 112 (b) Hazardous Air Pollutants (HAPs) : Not listed

Clean Air Act Section 602 Class I Substances : Not listed

Clean Air Act Section 602 Class II Substances : Not listed

DEA List I Chemicals (Precursor Chemicals) : Not listed

DEA List II Chemicals (Essential Chemicals) : Not listed

SARA 302/304

Composition/information on ingredients

No products were found.

SARA 304 RQ : Not applicable.

SARA 311/312

Classification : Sudden release of pressure

Composition/information on ingredients

Name	%	Fire hazard	Sudden release of pressure	Reactive	Immediate (acute) health hazard	Delayed (chronic) health hazard
Nitrogen	100	No.	Yes.	No.	No.	No.

Figure A.9: Safety Data Sheet for Nitrogen [49]

Nitrogen

Section 15. Regulatory information

State regulations

Massachusetts	: This material is listed.
New York	: This material is not listed.
New Jersey	: This material is listed.
Pennsylvania	: This material is listed.

International regulations

International lists

National inventory

Australia	: This material is listed or exempted.
Canada	: This material is listed or exempted.
China	: This material is listed or exempted.
Europe	: This material is listed or exempted.
Japan	: Not determined.
Malaysia	: Not determined.
New Zealand	: This material is listed or exempted.
Philippines	: This material is listed or exempted.
Republic of Korea	: This material is listed or exempted.
Taiwan	: This material is listed or exempted.

Canada

WHMIS (Canada) : Class A: Compressed gas.

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is not listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

Canada Label requirements : Class A: Compressed gas.

Hazardous Material Information System (U.S.A.)

Health	0
Flammability	0
Physical hazards	3

Caution: HMIS® ratings are based on a 0-4 rating scale, with 0 representing minimal hazards or risks, and 4 representing significant hazards or risks Although HMIS® ratings are not required on SDSs under 29 CFR 1910. 1200, the preparer may choose to provide them. HMIS® ratings are to be used with a fully implemented HMIS® program. HMIS® is a registered mark of the National Paint & Coatings Association (NPCA). HMIS® materials may be purchased exclusively from J. J. Keller (800) 327-6868.

The customer is responsible for determining the PPE code for this material.

National Fire Protection Association (U.S.A.)

Health

Flammability
Instability/Reactivity
Special

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Figure A.9: Safety Data Sheet for Nitrogen [49]

Section 16. Other information

Procedure used to derive the classification

Classification	Justification
Press. Gas Comp. Gas, H280	Expert judgment

History

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Key to abbreviations : ATE = Acute Toxicity Estimate
BCF = Bioconcentration Factor
GHS = Globally Harmonized System of Classification and Labelling of Chemicals
IATA = International Air Transport Association
IBC = Intermediate Bulk Container
IMDG = International Maritime Dangerous Goods
LogPow = logarithm of the octanol/water partition coefficient
MARPOL 73/78 = International Convention for the Prevention of Pollution From Ships, 1973 as modified by the Protocol of 1978. ("Marpol" = marine pollution)
UN = United Nations

References : Not available.

Indicates information that has changed from previously issued version.

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

Figure A.9: Safety Data Sheet for Nitrogen [49]

Phenolic Resin SDS

MOMENTIVE

Material Safety Data Sheet

FOR INDUSTRIAL USE ONLY

Cascophen RBS2345

1. Product and company identification

Product name	Cascophen RBS2345
MSDS Number	000000008613
Product Type	Phenol Formaldehyde Resin
Product use	Wood Adhesives, Composites, Laminates or Related Board Products
Manufacturer, Importer, Supplier	Momentive Specialty Chemicals Inc 180 East Broad Street Columbus OH 43215 4information@momentive.com
Print date	03-JAN-2011
Telephone	**For Emergency Medical Assistance** Call Health & Safety Information Services, 1-866-303-6949 **For Emergency Transportation Information** CHEMTREC US Domestic (800) 424-9300 CHEMTREC International (703) 527-3887 CANUTEC CA Domestic (613) 996-6666 For additional health and safety or regulatory information, call 1 888 443 9466 .

Part of the CASCO® Brand of Adhesives and Resins from Momentive Specialty Chemicals

2. Hazards identification

Form	Liquid
Odor	Slight aromatic
OSHA/HCS status	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
Emergency overview	WARNING ! CAUSES EYE IRRITATION. MAY CAUSE RESPIRATORY TRACT AND SKIN IRRITATION.

Potential acute health effects

Inhalation	Slightly irritating to the respiratory system. Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure.
Ingestion	Not expected to be harmful under normal conditions of use.
Skin	Slightly irritating to the skin.
Eyes	Severely irritating to eyes. Risk of serious damage to eyes.

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Figure A.10: Safety Data Sheet for Phenolic Resin SDS [13]

Potential chronic health effects

Chronic effects	No known significant effects or critical hazards.
Carcinogenicity	No known significant effects or critical hazards.
Mutagenicity	No known significant effects or critical hazards.
Teratogenicity	No known significant effects or critical hazards.
Developmental effects	No known significant effects or critical hazards.
Fertility effects	No known significant effects or critical hazards.
Target organs	Review Section 2 and 11 for any additional assessments.

Note: Residual formaldehyde gas may be released from this product during processing. The amount and level will depend on local conditions of use. Formaldehyde gas is irritating to the eyes and upper respiratory tract and may aggravate existing respiratory conditions or allergies. OSHA has listed formaldehyde as a potential human carcinogen. See the OSHA formaldehyde standard 29 CFR 1910.1048 for further details. The International Agency for Research on Cancer (IARC) has classified formaldehyde as carcinogenic to humans.

Over-exposure signs/symptoms

Inhalation	Adverse symptoms may include the following: respiratory tract irritation, coughing,
Ingestion	No specific data.
Skin	Adverse symptoms may include the following: irritation, redness,
Eyes	Adverse symptoms may include the following: pain or irritation, watering, redness,
Medical conditions aggravated by over-exposure	None known.

See section 11 for more detailed information on health effects and symptoms.

3. Composition/Information on ingredients

Ingredient name	CAS number	WT %
Phenol-Formaldehyde Polymer Sodium Salt	40798-65-0	**30.0 - 50.0**

*** Any applicable Canadian trade secret numbers will be listed in Section 15.*

4. First aid measures

Eye contact	Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Get medical attention. Chemical burns must be treated promptly by a physician.
Skin contact	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Continue to rinse for at least 10 minutes. Get medical attention if symptoms occur. Wash clothing before reuse. Clean shoes thoroughly before reuse.
Inhalation	Move exposed person to fresh air. Keep person warm and at rest. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide

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Figure A.10: Safety Data Sheet for Phenolic Resin SDS [13]

Large spill Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see section 13). Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Small spill Stop leak if without risk. Move containers from spill area. Dilute with water and mop up if water-soluble or absorb with an inert dry material and place in an appropriate waste disposal container. Dispose of via a licensed waste disposal contractor.

7. Handling and storage

Handling Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not breathe vapor or mist. Do not ingest. Avoid contact with eyes, skin and clothing. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Keep away from acids. Empty containers retain product residue and can be hazardous. Do not reuse container.

Storage Store in accordance with local regulations. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Separate from acids. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

8. Exposure controls/personal protection

Ingredient name	Occupational exposure limits

Consult local authorities for acceptable exposure limits.

Recommended monitoring procedures If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.

Engineering measures Use only with adequate ventilation. If user operations generate dust, fumes, gas, vapor or mist, use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.

Hygiene measures Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to

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Figure A.10: Safety Data Sheet for Phenolic Resin SDS [13]

the workstation location.

Respiratory	Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.
Hands	Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.
Eyes	Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.
Skin	Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Environmental exposure controls	Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

9. Physical and chemical properties

Form	Liquid
Flash point	Not applicable.
Auto-ignition temperature	Not applicable.
Flammable limits	
Lower:	Not applicable.
Upper:	Not applicable.
Color	Clear, reddish-brown
Odor	Slight aromatic
pH	11 - 12
Boiling point	Approx. 102 °C(216 °F)
Freezing Point	Less than 0 °C(32 °F)
Relative density	Approx. 1.1750 - 1.1950
Vapor pressure	Approx. 22 mm Hg @ 25 °C(77 °F)
Odor threshold	Not available
Viscosity	Dynamic- 1,200 - 1,800 cPs Brookfield
Solubility	Infinite
Partition coefficient: n-octanol/water	Not available
Evaporation rate	Approx. 0.4 (n-Butyl acetate=1)
Vapor density	Not available
Typical % solids	41.00 % (m)

10. Stability and reactivity

Stability	Hazardous polymerization may occur under certain conditions of storage or use.
Conditions to avoid	Strong oxidizer.

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Figure A.10: Safety Data Sheet for Phenolic Resin SDS [13]

artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if adverse health effects persist or are severe. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.

Ingestion	Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.
Protection of first aid personnel	No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.
Notes to physician	In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.

See section 11 for more detailed information on health effects and symptoms.

5. Fire-fighting measures

Flammability of the product	In a fire or if heated, a pressure increase will occur and the container may burst.
Extinguishing media	
Suitable	Use an extinguishing agent suitable for the surrounding fire.
Not suitable	None known.
Special exposure hazards	Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training.
Hazardous combustion products	Decomposition products may include the following materials: carbon oxides, nitrogen oxides.
Special protective equipment for fire-fighters	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

6. Accidental release measures

Personal precautions	No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 8).
Environmental precautions	Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

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Figure A.10: Safety Data Sheet for Phenolic Resin SDS [13]

Materials to avoid — Reactive or incompatible with the following materials: oxidizing materials, acids,

Hazardous decomposition products — Decomposition products may include the following materials: carbon monoxide, carbon dioxide, aldehydes (including formaldehyde), oxides of nitrogen particulate matter, other organic compounds,

11. Toxicological information

Acute toxicity
Product name
Cascophen RBS2345

LC50 Inhalation	Rat	> 2501 ppm/1 hEstimated
16 CFR Part 1500.41	Rabbit	Slight Skin Irritant
16 CFR Part 1500.42	Rabbit	Severe Eye Irritant

Acute toxicity
Ingredient name

Other Toxicological Information

Carcinogenicity
Classification
Ingredient name
Phenol-Formaldehyde Polymer Sodium Salt

ACGIH	Not classified
IARC	Not classified
NTP	Not listed
OSHA	Not regulated
EU	Not classified

12. Ecological information

Environmental effects
No known significant effects or critical hazards.

Biodegradability
Conclusion/Summary — Phenol-formaldehyde polymers have a very low rate of biodegradation.

Other adverse effects
Bioaccumulation is expected to be minimal. Product is initially a mobile liquid which will solidify on aging. Unreacted monomer may be leached into ground water even after normal curing has occurred.

13. Disposal considerations

Waste disposal — The generation of waste should be avoided or minimized wherever possible. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

14. Transport information

The data provided in this section is for information only and may not be specific to your package size or mode of transport. You will need to apply the appropriate regulations to properly classify your shipment for transportation.

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Figure A.10: Safety Data Sheet for Phenolic Resin SDS [13]

International transport regulations

Regulatory information	UN/NA number	Proper shipping name	Classes/*PG	Reportable Quantity (RQ)
CFR		Non-regulated		
TDG		Non-regulated		
IMO/IMDG		Non-regulated		
IATA (Cargo)		Non-regulated		

*PG : Packing group

15. Regulatory information

US regulations

HCS Classification Irritating material

U.S. Federal regulations

SARA 311/312 Classification Immediate (acute) health hazard, reactive

SARA 313 - Supplier Notification
This product contains the following toxic chemical(s) subject to the reporting requirements of Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986, and Subpart C-Supplier Notification Requirement of 40 CFR Part 372.
None required.

SARA 302 Extremely Hazardous Substances None required.

State regulations

Massachusetts RTK Substances None required.

New Jersey RTK Hazardous Substances None required.

Pennsylvania RTK Hazardous Substances None required.

California Prop. 65: WARNING: This product contains a chemical known to the State of California to cause cancer. Formaldehyde - 50-00-0.

Canada

WHMIS (Canada) Class D-2A: Material causing other toxic effects (Very toxic).

Canadian lists **Canadian NPRI**: None required.

International regulations

Chemical inventories

Europe inventory All components are listed or exempted.
Australia inventory (AICS) Not determined.
China inventory (IECSC) Not determined.
Japan inventory (ENCS) Not determined.
Japan inventory (ISHL) Not determined.
Korea inventory (KECI) Not determined.
New Zealand Inventory (NZIoC) Not determined.
Philippines inventory (PICCS) Not determined.
United States inventory (TSCA 8b) All components are listed or exempted.
Canada inventory All components are listed or exempted.

16. Other information

Hazardous Material Health : 2

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Figure A.10: Safety Data Sheet for Phenolic Resin SDS [13]

Information System III (U.S.A.)	Flammability: 0 Physical hazards : 0 Chronic :

Caution: HMIS® ratings are based on a 0-4 rating scale, with 0 representing minimal hazards or risks, and 4 representing significant hazards or risks Although HMIS® ratings are not required on MSDSs under 29 CFR 1910.1200, the preparer may choose to provide them. HMIS® ratings are to be used with a fully implemented HMIS® program. HMIS® is a registered mark of the National Paint & Coatings Association (NPCA). HMIS® materials may be purchased exclusively from J. J. Keller (800) 327-6868.
The customer is responsible for determining the PPE code for this material.

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Figure A.10: Safety Data Sheet for Phenolic Resin SDS [13]