MEMORANDUM

Date: March 9, 2017

To: Tiffany Rau, Design Competition Chair, AIChE
Chelsea Monty, Design Competition Chair, AIChE
Sarah Ewing, Student Project Lead, AIChE

From: Design Group:

Subject: Proposed Manufacturing Facility for Nylon 6,6

This memorandum is in response to the proposed nylon 6,6 manufacturing facility in Calvert City, Kentucky. The team was tasked with designing a polymerization process to annually produce 85 million pounds of nylon 6,6 by reacting adipic acid and hexamethylene diamine. The team was also tasked with investigating a turndown case which operates at 67% of full capacity. The produced nylon 6,6 was either granulated or spun into fibers. This decision was made based on the most economically attractive option. A waste water stream and a gas stream were two by-product streams. The waste water was sent off site for treatment and the gas stream was sent through a scrubber and vented to the atmosphere. Project construction will finish by the end of 2017. Production will begin at the start of 2018.

The design report enclosed covers both the full production case and a turndown case which operates at 67% of full capacity with technical analysis and economic considerations. An appendix with detailed design methods is also included.

Sincerely,
Design Group:

Proposed Manufacturing Facility for Nylon 6,6

March 9, 2017

Team #________

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Abstract:

The purpose of this project was to design an economically viable process that produces 85 million pounds of nylon 6,6 annually. This process would be carried out in a new plant that would be built in the Calvert City, Kentucky area. The full capacity fiber design achieves this production goal and produces nylon 6,6 with a number average molecular weight of 2635 amu and an average degree of polymerization of 23.3 monomers per molecule.

The production of nylon 6,6 fibers was determined to be more economically attractive than granular nylon 6,6 due to its much larger net present value (NPV) of approximately $174 million compared to the granular NPV of negative $190 million. The production of nylon 6,6 fibers had a discount cash flow rate of return (DCFROR) of 243% and a discounted payback period of only 6 months. The production of nylon 6,6 fibers is still economically attractive and physically feasible under turndown conditions with an NPV of approximately $98 million, a DCFROR of 145%, and a discounted payback period of 10 months. The turndown period does have a slightly higher cost of manufacturing per pound of nylon 6,6 produced, costing $1.59 per pound as opposed to the $1.51 per pound that full scale production costs. It is recommended that the design to produce nylon 6,6 fiber is carried forward to the detailed design stage and operated at full capacity.

The reaction was simulated in Polymath using two key assumptions. The reaction was carried out at 72.5 psig and 622°F while the vapor pressure of water under these conditions was greater than 1400 psig. This discrepancy in reactor pressure and vapor pressure led to the assumption that the water produced by the condensation polymerization reaction and the water introduced by the feed stream instantly vaporizes and it is vented from the reactor. HMDA is significantly less volatile than water and was assumed to be non-volatile under reaction conditions. The 72.5 psig reaction pressure was chosen to help justify this assumption without impacting capital costs significantly. Further investigation into these two assumptions and the effects of deviations from the simulation model are recommended.

Introduction:

Synthetic polymers are a substantial part of the textile and plastic industries. One of the most important classes of synthetic polymers are polyamides, also known as nylon. Two of the of most commonly used polyamides are nylon 6 and nylon 6,6. Nylon 6,6 will be the focus of this report. With the growing demand in Europe for light weight vehicles, of which nylon 6,6 is a major component, the market for nylon 6,6 is expected to increase in the coming years. There is also an increasing demand for light weight, high performance materials for electronics which will further drive the market up. Due to such a wide use and demand for this polymer, it is clear that there is potential profit in this venture [30]. Nylon 6,6 is a co-polymer that is produced from the step-growth polymerization of adipic acid and hexamethylene diamine (HMDA). The number designation for nylon 6,6 comes from the fact that the two monomers each have 6 carbon atoms. Nylon 6,6 can be produced through the polycondensation of HMDA and adipic acid. The adipic acid and HMDA are combined with water in a reactor to produce nylon 6,6 salt. This salt will be polymerized in a reaction vessel, forming nylon 6,6 [20].

The main objective of this project is to design a manufacturing facility for nylon 6,6 in Calvert City, Kentucky that produces 85 million pounds of nylon 6,6 per year. The industrial process will be designed to operate at full capacity. Additionally, the process will be analyzed at a reduced capacity of 67% to ensure the plant can safely operate in the event of a reduced demand. The process will either be a batch or continuous process where the final product will take the form of granules or fibers. The process will not only generate a product stream, but also two side product streams which will be taken into account in the process design and in the economic analysis. Economic analyses will be performed for both the full capacity and reduced capacity cases. These economic analyses will be performed with an internal rate of return of 15% and an effective tax rate of 40%. This project will be evaluated over 10-years where the equipment will be depreciated using MACRS depreciation. For the purpose of the economic evaluation, construction will begin immediately and finish at the end of 2017 with startup occurring at the beginning of 2018.

The following report will include the finished process design; important safety, health, and environmental considerations; an economic evaluation of the process; and overall conclusions and recommendations.

Process Flow Diagram and Material Balances:

The process flow diagrams and stream summary table for the full capacity case and the reduced capacity case can be found on pages 3-8.

R-101	R-102	R-103	R-104	R-105	R-106	R-107	V-101	V-102	E-101	E-102	E-103	E-104	E-105	P-101A/B	P-102A/B
Aqueous HMDA Mixer	Nylon Salt Reactor	First Poly. Reactor	Second Poly. Reactor	Third Poly. Reactor	Fourth Poly. Reactor	Fifth Poly. Reactor	Nylon Salt Receiver	Condensate Receiver	DI Water Heater	Water Recycle Condenser	Water Recycle Cooler	Falling Film Evaporator	Nylon 6,6 Melt Cooler	DI Water Pump	Aqueous HMDA pump

P-103A/B	P-104A/B	P-105A/B	P-106A/B	P-107A/B	P-108A/B	P-109A/B	P-110A/B	X-102	X-103	X-104	X-105	X-106
Pump to Nylon Salt Receiver	Pump to Evaporator	Pump to Poly. Reactor 1	Pump to Poly. Reactor 2	Pump to Poly. Reactor 3	Pump to Poly. Reactor 4	Pump to Poly. Reactor 5	Water Recycle Pump	Adipic Acid Conveyor	HMDA Conveyor	Solid Adipic Acid Hopper	Solid HMDA Hopper	Yarn Extruders

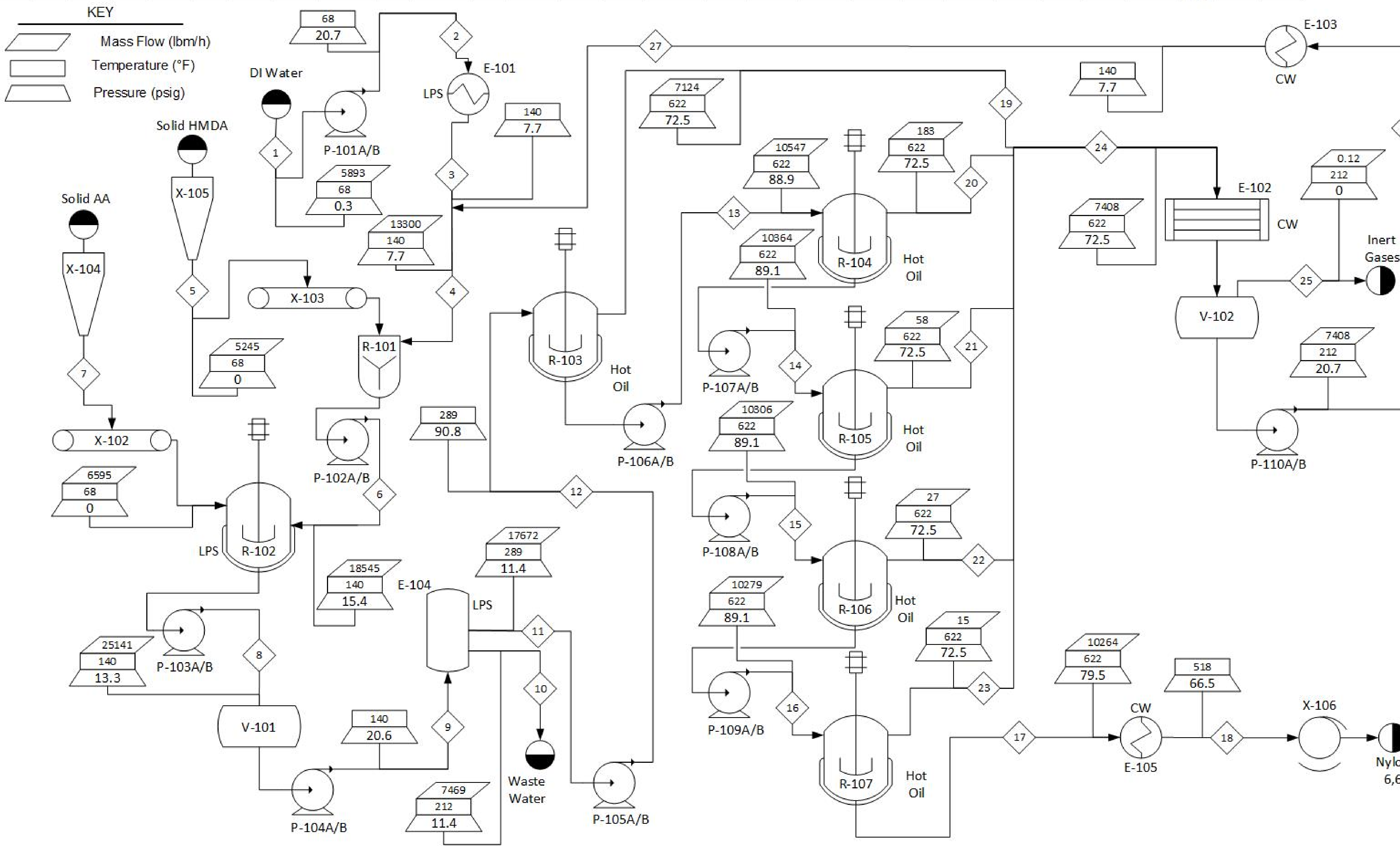

Figure 1: Full Nylon 6,6 Fiber Production PFD

Table 1: Streams 1-14 Summary Table for Full Nylon 6,6 Fiber Production

Stream Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Stream Description	**DI Water Feed**	**To E-101**	**From E-101**	**To R-101**	**To X-103**	**To R-102**	**To X-102**	**To V-101**	**To E-104**	**Evaporated Water Stream**	**From E-104**	**To R-103**	**To R-104**	**To R-105**
Temperature (°F)	68	68	140	140	68	140	68	140	140	212	289.4	289.4	622.4	622.4
Pressure (psig)	0.3	20.7	7.7	7.7	0.0	15.4	0.0	13.3	20.6	11.4	11.4	90.8	88.9	89.1
Vapor Fraction	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mass Flow (lb/hr)	5893	5893	5893	13300	5245	18545	6595	25141	25141	7469	17672	17672	10547	10364
Molar Flow (lbmol/hr)	327.0	327.0	327.0	738.1	45.1	783.4	45.1	783.4	783.4	414.5	368.8	368.8	20.3	9.6
Component Mole Fraction	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Water	1.00	1.00	1.00	1.00	0.00	0.94	0.00	0.94	0.94	1.00	0.88	0.88	0.00	0.00
Hexamethylene diamine	0.00	0.00	0.00	0.00	1.00	0.06	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Adipic Acid	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nylon Salt	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.06	0.00	0.12	0.12	0.00	0.00
Nylon 6,6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	1.00
Ammonium	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Carbon Dioxide	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Actual Volume Flow (ft^3/hr)	94.4	94.4	94.4	213.1	100.0	315.1	77.7	395.1	395.1	124.8	291.5	291.5	191.1	180.2
Density (lb/ft^3)	62.40	62.40	62.40	62.40	52.44	58.85	84.90	63.63	63.63	59.83	60.62	60.62	55.20	57.50
Molecular Weight	18.02	18.02	18.02	18.02	116.21	23.67	146.14	32.09	32.09	18.02	47.91	47.91	520.70	1082.63

Table 2: Streams 15-27 Summary Table for Full Nylon 6,6 Fiber Production

Stream Number	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**
Stream Description	**To R-106**	**To R-107**	**To E-105**	**To X-105**	**R-103 Vent**	**R-104 Vent**	**R-105 Vent**	**R-106 Vent**	**R-107 Vent**	**To E-102**	**Inert Gas Vent**	**To E-103**	**Water Recycle Stream**
Temperature (°F)	622.4	622.4	622.4	518	622.4	622.4	622.4	622.4	622.4	622.4	212	212	140
Pressure (psig)	89.1	89.1	79.5	66.5	72.5	72.5	72.5	72.5	72.5	72.5	0	20.7	7.7
Vapor Fraction	0	0	0	0	1	1	1	1	1	1	1	0	0
Mass Flow (lb/hr)	10306	10279	10264	10264	7124	183	58	27	15	7407.67	0.12	7407.55	7407.55
Molar Flow (lbmol/hr)	6.3	4.8	3.9	3.9	395.4	10.2	3.2	1.5	0.9	411.1	0.004	411.1	411.1
Component Mole Fraction	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Water	0.00	0.00	0.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	1.00
Hexamethylene diamine	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Adipic Acid	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nylon Salt	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nylon 6,6	1.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ammonium	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.67	0.00	0.00
Carbon Dioxide	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.33	0.00	0.00
Actual Volume Flow (ft^3/hr)	176.8	175.2	174.3	167.8	62353.4	1604.0	505.2	235.9	134.6	64833.1	1.3	123.8	120.7
Density (lb/ft^3)	58.28	58.66	58.88	61.16	0.11	0.11	0.11	0.11	0.11	0.11	0.09	59.83	61.38
Molecular Weight	1640.82	2161.76	2634.56	2634.56	18.02	18.02	18.02	18.02	18.02	18.02	26.04	18.02	18.02

R-101	R-102	R-103	R-104	R-105	R-106	R-107	V-101	V-102	E-101	E-102	E-103	E-104	E-105	P-101A/B	P-102A/B	P-103A/B	P-104A/B	P-105A/B	P-106A/B	P-107A/B	P-108A/B	P-109A/B	P-110A/B	X-102	X-103	X-104	X-105	X-106
Aqueous HMDA Mixer	Nylon Salt Reactor	First Poly. Reactor	Second Poly. Reactor	Third Poly. Reactor	Fourth Poly. Reactor	Fifth Poly. Reactor	Nylon Salt Receiver	Condensate Receiver	DI Water Heater	Water Recycle Condenser	Water Recycle Cooler	Falling Film Evaporator	Nylon 6,6 Melt Cooler	DI Water Pump	Aqueous HMDA pump	Pump to Nylon Salt Receiver	Pump to Evaporator	Pump to Poly. Reactor 1	Pump to Poly. Reactor 2	Pump to Poly. Reactor 3	Pump to Poly. Reactor 4	Pump to Poly. Reactor 5	Water Recycle Pump	Adipic Acid Conveyor	HMDA Conveyor	Solid Adipic Acid Hopper	Solid HMDA Hopper	Yarn Extruders

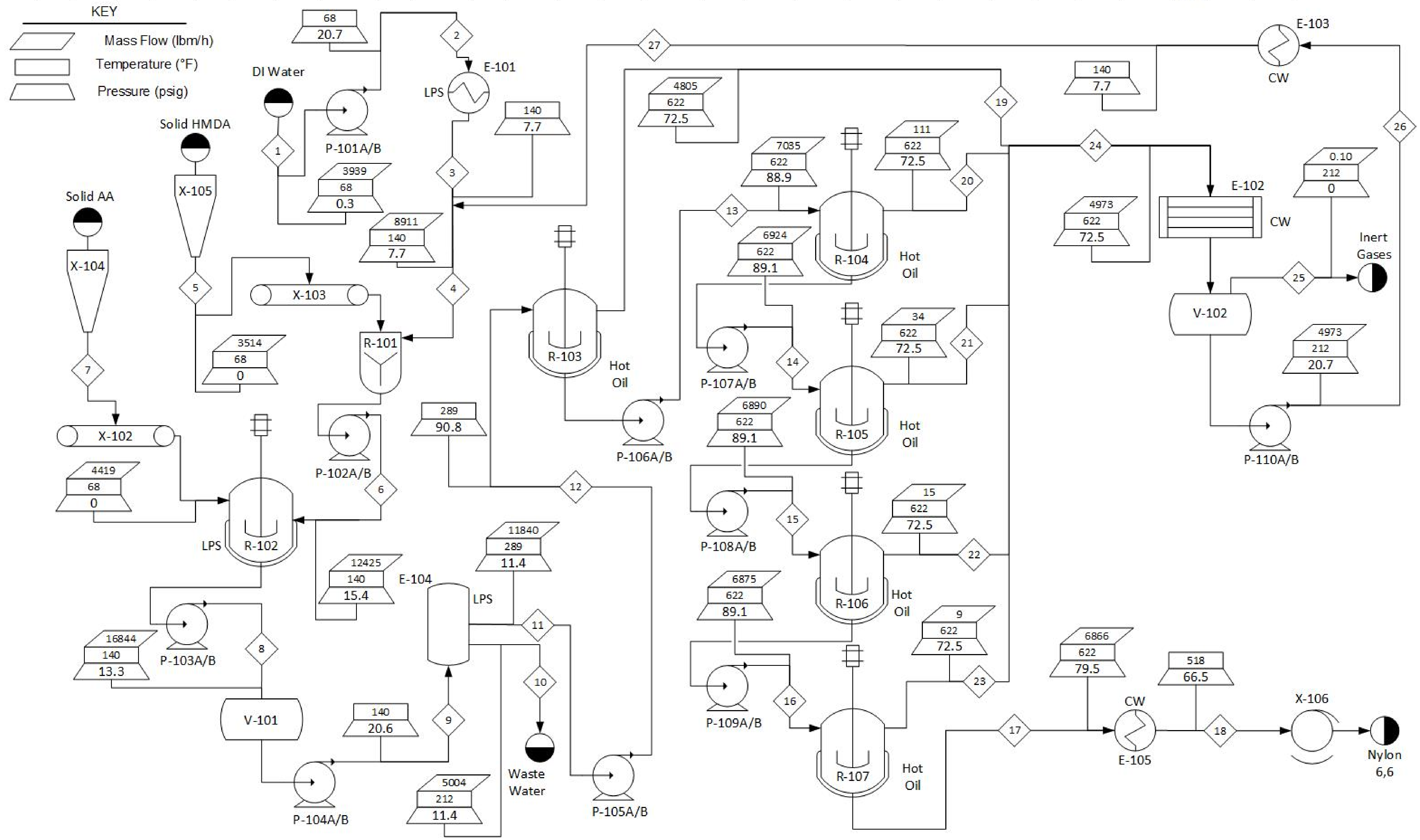

Figure 2: Turndown Nylon 6,6 Production PFD

Table 3: Streams 1-14 Summary Table for Turndown Nylon 6,6 Production

Stream Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Stream Description	**DI Water Feed**	**To E-101**	**From E-101**	**To R-101**	**To X-103**	**To R-102**	**To X-102**	**To V-101**	**To E-104**	**Evaporated Water Stream**	**From E-104**	**To R-103**	**To R-104**	**To R-105**
Temperature (°F)	68	68	140	140	68	140	68	140	140	212	289.4	289.4	622.4	622.4
Pressure (psig)	0.3	20.7	7.7	7.7	0.0	15.4	0.0	13.3	20.6	11.4	11.4	90.8	88.9	89.1
Vapor Fraction	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mass Flow (lb/hr)	3939	3939	3939	8911	3514	12425	4419	16844	16844	5004	11840	11840	7035	6924
Molar Flow (lbmol/hr)	218.6	218.6	218.6	494.5	30.2	524.9	30.2	524.9	524.9	277.7	247.1	247.1	11.7	5.4
Component Mole Fraction	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Water	1.00	1.00	1.00	1.00	0.00	0.94	0.00	0.94	0.94	1.00	0.88	0.88	0.00	0.00
Hexamethylene diamine	0.00	0.00	0.00	0.00	1.00	0.06	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Adipic Acid	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nylon Salt	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.06	0.00	0.12	0.12	0.00	0.00
Nylon 6,6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	1.00
Ammonium	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Carbon Dioxide	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Actual Volume Flow (ft^3/hr)	63.1	63.1	63.1	142.8	67.0	211.1	52.0	264.7	264.7	83.6	195.3	195.3	126.2	119.6
Density (lb/ft^3)	62.40	62.40	62.40	62.40	52.44	58.85	84.90	63.63	63.63	59.83	60.62	60.62	55.76	57.91
Molecular Weight	18.02	18.02	18.02	18.02	116.21	23.67	146.14	32.09	32.09	18.02	47.91	47.91	599.67	1290.14

Table 4: Streams 15-27 Summary Table for Turndown Nylon 6,6 Production

Stream Number	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**
Stream Description	**To R-106**	**To R-107**	**To E-105**	**To X-105**	**R-103 Vent**	**R-104 Vent**	**R-105 Vent**	**R-106 Vent**	**R-107 Vent**	**To E-102**	**Inert Gas Vent**	**To E-103**	**Water Recycle Stream**
Temperature (°F)	622.4	622.4	622.4	518	622.4	622.4	622.4	622.4	622.4	622.4	212	212	140
Pressure (psig)	89.1	89.1	79.5	66.5	72.5	72.5	72.5	72.5	72.5	72.5	0	20.7	7.7
Vapor Fraction	0	0	0	0	1	1	1	1	1	1	1	0	0
Mass Flow (lb/hr)	6890	6875	6866	6866	4805	111	34	15	9	4973	0.10	4973	4973
Molar Flow (lbmol/hr)	3.5	2.6	2.1	2.1	266.6	6.2	1.9	0.8	0.5	276.0	0.004	276.0	276.0
Component Mole Fraction	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Water	0.00	0.00	0.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	0.00	1.00	1.00
Hexamethylene diamine	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Adipic Acid	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nylon Salt	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nylon 6,6	1.00	1.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ammonium	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.67	0.00	0.00
Carbon Dioxide	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.33	0.00	0.00
Actual Volume Flow (ft^3/hr)	117.6	116.7	116.2	112.1	42050.8	970.6	293.3	132.5	75.9	43522.9	1.1	83.1	81.0
Density (lb/ft^3)	58.59	58.90	59.08	61.28	0.11 [26]	0.11 [26]	0.11 [26]	0.11 [26]	0.11 [26]	0.11 [26]	0.09	59.83	61.38
Molecular Weight	1987.81	2629.82	3225.71	3225.71	18.02	18.02	18.02	18.02	18.02	18.02	26.03	18.02	18.02

Process Description:

HMDA powder for this process is stored in a hopper and is discharged out of the bottom onto a conveyer belt where it is taken to a mixer and mixed with heated deionized water. After the stream leaves the mixer, it is sent to a continuous stirred-tank reactor (CSTR) where the HMDA in the stream is reacted with solid adipic acid to form nylon 6,6 salt. The salt is pumped into a holdup tank. The salt solution is then pumped into an evaporator to remove some of the water. After the solution leaves the evaporator it is pumped into a series of five jacketed CSTRs where it is heated to 622 °F and the polymerization reaction occurs. The CSTR are heated by running hot oil through their jackets. During the reaction, the water that was present in the feed stream is vaporized and vented out of the tops of the CSTRs. The carbon dioxide, ammonia, and water that is formed during the polymerization reaction and the accompanying degradation reactions are also vented out of the tops of the CSTRs. Once the nylon 6,6 salt has travelled through the five CSTRs, it exits as nylon 6,6. The nylon 6,6 is pumped through a cooler to aid with the extrusion and is then sent through extruders which produces nylon 6,6 fibers. The vapors that are vented out of the CSTRs are combined into a single stream and sent to a condenser. The condenser lowers the temperature of the stream until the water in the stream condenses. After exiting the condenser, the steam is sent to a condensate receiver tank which acts as a flash drum, separating the carbon dioxide and ammonia from the water. The carbon dioxide/ammonia stream then exits the process and is sent to a scrubber. The condensed water stream is cooled and returned as a recycle stream to be mixed with the HMDA feed at the beginning of the process. The Process Flow Diagram for this process can be seen on page 3. The stream summary tables indicating the properties for the streams in the process can be seen on pages 4 and 5.

The HMDA was mixed with water prior to entering the salt reactor because HMDA is known to be hazardous in solid form [24]. Mixing it with water as early as possible reduces the potential for worker injury due to exposure to particulate HMDA. An evaporator was used before the polymerization CSTRs because the presence of water slows down the polymerization reaction. Removing the water before the stream enters the reactors reduces the amount of water present that will inhibit the polymerization reaction [27]. The exact pressure of the polymerization reactors was chosen based on keeping the pressure as high as possible without incurring additional capital costs associated with high pressure equipment [31]. Higher pressure was desired in order to minimize the amount of HMDA exiting the reactors as a vapor. This was important because the developed model does not take into account the evaporation of HMDA, and the system is known to be sensitive to changes in the stoichiometric ratio of HMDA and adipic acid. CSTRs were chosen over other reactor types because CSTRs allow water to be removed from the reactor while the reaction is taking place, which pushes the reaction equilibrium towards the desired product [20]. This is not true of plug flow reactors and most other reactor types. An exception to this would be a semi batch reactor. CSTRs were chosen over semi batch reactors because a continuous process reduces the amount of chemical intermediates that need to be stored at any given time. A continuous process is also known to produce a narrower molecular weight distribution among polymers, making a more consistent product [11]. In general, continuous processes are also more easily controlled than batch processes. The reactors were heated up to 622 °F because a survey of the literature regarding the process indicated that 440°F to 620 °F is standard, and 622 °F is approximately 18°F lower than the maximum temperature hot oil can be heated to [7][18][6]. This allows for an 18 °F difference between the heating element and the process fluid. The maximum temperature was chosen because the reaction kinetics become more favorable at higher temperatures [18]. Hot oil was used as the heating medium because high pressure steam would not be capable of getting the reactors up to the required temperature [31]. Pumps were placed between the polymerization CSTRs to overcome line losses and any static head caused by the physical layout of the system. The heat exchanger located before the extruder cools the nylon 6,6 stream in order to make the extruders more effective [33].

Energy Balance and Utility Requirements:

This design of nylon 6,6 production involves multiple energy consuming pieces of equipment. In total there are 4 shell-and-tube heat-exchangers, 1 falling-film evaporator, 6 jacketed reactors, and one furnace that all use heat transfer materials. There are also 10 pumps and 7 impeller stirrers that consume electricity within this process. Although there are hoppers with electrically controlled extruders and conveyor belts included in this process, their associated electrical consumption was considered negligible. The utilities used to meet the energy requirements of the equipment are summarized in Table 5.

Table 5: Process Utility Origins

Utility	Vehicle
Electricity	Purchased from off-site power station, transferred to site by means of transmission lines
Low Pressure Steam (LPS)	Made by on-site steam boiler
Cooling Water (CW)	Made by on-site cooling water tower
Natural Gas (NG)	Purchased from off-site source, transferred to site by means of gas lines
Wastewater Treatment (WWT)	Water sent to off-site wastewater treatment facility by means of water lines
Hot Oil	Duratherm HF-FG heated in on-site hot oil furnace (X-101)

The capital costs associated with the vehicles of utility delivery are included in the grassroots capital cost correlations for the process equipment and thus are not calculated on their own [31]. The demand for these utilities was determined through the use of energy balances or selected engineering heuristics on the individual pieces of equipment that require their use. Equations 1-8 was used to determine the individual equipment energy requirements.

Shell-and-tube heat-exchangers:

$$\dot{m}_{LPS} = \frac{\dot{Q}}{\Delta H_{vap}} \qquad \textit{Equation 1}$$

Where,

$\dot{m}_{LPS}$ = the mass flowrate of the low pressure steam being condensed in the heat-exchanger

$\dot{Q}$ = the required heat transfer rate to the product stream in order to achieve desired temperature change

ΔH_{vap} = the heat of vaporization of the low pressure steam

$$\dot{m}_{CW} = \frac{\dot{Q}}{C_p \Delta T} \quad \textit{Equation 2}$$

Where,

$\dot{m}_{CW}$ = the mass flowrate of the cooling water flowing through the heat-exchanger

$\dot{Q}$ = the required heat transfer rate to cooling water stream in order to achieve required temperature change in the product sream

C_p = the specific heat of the cooling water

ΔT = the difference in temperature of the inlet and outlet cooling water conditions

Falling-film evaporator:

$$\dot{m}_{LPS} = \frac{\dot{Q}}{\Delta H_{vap}} \quad \textit{Equation 3}$$

Where,

$\dot{m}_{LPS}$ = the mass flowrate of the low pressure steam being condensed in the heat-exchanger

$\dot{Q}$ = the required heat transfer rate to the product stream in order to achieve desired temperature change

ΔH_{vap} = the heat of vaporization of the low pressure steam

$$F_{wastewater} = \frac{\dot{m}_{evap}}{\rho_{water}} \quad \textit{Equation 4}$$

Where,

$\dot{m}_{wastewater}$ = the mass of the water that will be sent to wastewater treatment

$\dot{m}_{evap}$ = the mass of water being evaporated out of the product stream

ρ_{water} = the density of water at STP

Jacketed Reactor:

$$\dot{m}_{LPS} = \frac{\dot{Q}}{\Delta H_{vap}} \quad \textit{Equation 5}$$

Where,

$\dot{m}_{LPS}$ = the mass flowrate of the low pressure steam being condensed in the jacket of the reactor

$\dot{Q}$ = the required heat transfer rate to the reactor in order to maintain specified temperature

ΔH_{vap} = the heat of vaporization of the low pressure steam

Furnace:

$$\dot{Q}_{NG} = \sum \dot{Q}_{Reactors} \quad \textit{Equation 6}$$

Where,

$\dot{Q}_{NG}$ = the heat transfer flowrate required from natural gas flowing through the furnace

$\dot{Q}_{Reactors}$ = the heat transfer rate requirement for jacketed reactors that use Duratherm as its heat transfer material

Pumps:

$$hp_{purchased} = \frac{bhp}{\varepsilon_{motor}} \quad \textit{Equation 7}$$

Where,

$hp_{purchased}$ = purchased horsepower

bhp = break horsepower

ε_{motor} = motor efficiency

Impeller stirrer:

$$P_{Required} = F * P_{Coefficent} \quad \textit{Equation 8}$$

Where,

$P_{Required}$ = the power requirement to operate the stirrer

F = the flowrate out of the reactor

$P_{Coefficent}$ = the mixing parameter based on type of fluid inside reactor [12]

The heat transfer fluid, Duratherm, is recycled and thus is not steadily consumed like the natural gas and electricity. The price of the Duratherm is accounted for in the working capital of the plant. The cost of heating the Duratherm in the furnace is accounted for in the cost of the natural gas consumed by the furnace.

Table 6 is a summary of the required utilities for each piece of equipment that consumes a utility.

Table 6: Utility Usage

Equipment	Electricity (kWh/yr)	LPS (lbm/yr)	CW (m^3/yr)	NG (GJ/yr)	WWT (m^3/yr)
R-101	2.19E+04				
R-102	2.75E+04	3.63E+06			
R-103	1.33E+04				
R-104	1.25E+04				
R-105	1.23E+04				
R-106	1.22E+04				
R-107	1.22E+04				
E-101		8.28E+06			
E-102			2.61E+05		
E-103			3.84E+04		
E-104		6.39E+07			2.82E+04
E-105			3.87E+03		
P-101	8.27E+03				
P-102	8.27E+03				
P-103	6.33E+03				
P-104	1.58E+04				
P-105	1.08E+05				
P-106	1.08E+05				
P-107	1.08E+05				
P-108	1.08E+05				
P-109	1.08E+05				
P-110	4.35E+03				
P-111	4.35E+03				
P-112	4.35E+03				
P-113	4.35E+03				
P-114	4.35E+03				
X-101				2.53E+04	
X-106	1.12E+07				

The decision was made to recycle the water that is being vented off of R-103, R-104, R105, R-106 and R-107 back into R-101 in order to reduce the amount of wastewater being produced and the amount of deionized water needed. Due to the higher price of low pressure steam compared to cooling water, it is less expensive to condense and cool the water being vented than it is to heat the extra deionized water that would be required if the recycle stream were not in place.

The annual requirement and cost of these purchased utilities, including wastewater treatment is shown in Table 7.

Table 7: Annual Utility Costs

Ultility	Ultility Price	Annual Required Quantity	Annual Cost
Electricity	\$/kWh	kWh/yr	\$712,738
	0.060	1.19E+07	
Cooling Water	\$/m^3	m^3/yr	\$4,494
	0.015	3.04E+05	
Low Pressure Steam	\$/lbm	lbm/yr	\$944,076
	0.013	7.11E+07	
Natural Gas	\$/GJ	GJ/yr	\$280,735
	11.1	2.53E+04	
Wastewater Treatment	\$/m^3	m^3/yr	\$1,156
	0.041	2.82E+04	

Equipment List and Unit Descriptions:

Table 8 is a list of the names and descriptions of the process equipment.

Table 8: Equipment List

Unit #	Unit Type	Function	M.O.C	Size	Operating Temperature (F)	Operating Pressure (psig)
R-101	Jacketed Vessel	Aqueous HMDA Mixer	SS	5.91 m^3	140	0
R-102	Jacketed Vessel	Nylon Salt Reactor	SS	9.32 m^3	140	0
R-103	Jacketed Vessel	First Polymerization Reactor	SS	26.8 m^3	622.4	72.5
R-104	Jacketed Vessel	Second Polymerization Reactor	SS	17.6 m^3	622.4	72.5
R-105	Jacketed Vessel	Third Polymerization Reactor	SS	16.6 m^3	622.4	72.5
R-106	Jacketed Vessel	Fourth Polymerization Reactor	SS	16.3 m^3	622.4	72.5
R-107	Jacketed Vessel	Fifth Polymerization Reactor	SS	16.1 m^3	622.4	72.5
V-101	Horizontal Process Vessel	Nylon Salt Receiver	SS	2.29 m^3	140	0
V-102	Horizontal Process Vessel	Condensate Receiver	SS	.760 m^3	212	0
E-101	Shell-and-Tube Heat-Exchanger	Deionized Water Heater	CS	2.70 m^2	320	72.5
E-102	Shell-and-Tube Heat-Exchanger	Water Recycle Condenser	SS	20.6 m^2	622.4	72.5
E-103	Shell-and-Tube Heat-Exchanger	Water Recycle Cooler	SS	5.16 m^2	212	20.7
E-104	Falling-Film Evaporator	Nylon Salt Feed Evaporator	SS	7.80 m^2	320	72.5
E-105	Shell-and-Tube Heat-Exchanger	Nylon 6,6 Melt Cooler	SS	.909 m^2	622.4	79.5
P-101	Centrifugal Pump	Deionized Water Feed Pump	CS	.746 kW	68	20.7
P-102	Centrifugal Pump	Aqueous HMDA Pump	SS	.746 kW	140	15.4
P-103	Centrifugal Pump	Pump to Nylon Salt Receiver	SS	.559 kW	140	13.3
P-104	Centrifugal Pump	Pump to Evaporator	SS	1.49 kW	140	20.6
P-105	Centrifugal Pump	Pump to First Polymerization Reactor	SS	3.73 kW	289.4	90.8
P-106	Centrifugal Pump	Pump Second Polymerization Reactor	SS	0.373 kW	622.4	88.9
P-107	Centrifugal Pump	Pump to Third Polymerization Reactor	SS	0.373 kW	622.4	89.1
P-108	Centrifugal Pump	Pump to Fourth Polymerization Reactor	SS	0.373 kW	622.4	89.1
P-109	Centrifugal Pump	Pump to Fifth Polymerization Reactor	SS	0.373 kW	622.4	89.1
P-110	Centrifugal Pump	Water Recycle Pump	SS	0.373 kW	140	20.7
X-101	Furnace	Duratherm Furnace	CS	844 kW	640.4	0
X-102	Conveyor	Adipic Acid Conveyor	SS	.0117 m^2	68	0
X-103	Conveyor	HMDA Conveyor	SS	.0189 m^2	68	0
X-104	Hopper	Solid Adipic Acid Hopper	SS	.193 m^3 [29]	68	0
X-105	Hooper	Solid HMDA Hopper	SS	.193 m^3 [29]	68	0
X-106	Extruder	Nylon 6,6 Yarn Extruders	SS	33.6 m^2 [1]	518	66.5

R-101

The volume of R-101, the mixer that combines deionized water and HMDA into an aqueous solution to be pumped into R-102, was calculated using the following equation:

$$V = v_0 * (\tau + t_{surge}) \quad \textit{Equation 9}$$

Where,

V = the volume of the reactor

v_0 = the volumetric flowrate into the reactor

τ = the residence time of reactor

t_{surge} = the determined surge time of the reactor

The mixture of HMDA and deionized water was assumed to be ideal in order to calculate the volumetric flowrate entering the mixer. This volumetric flowrate was determined using the required mass flowrate and densities of HMDA and water. The amount of water introduced into the mixer is controlled to produce a nylon 6,6 salt solution that is completely soluble in water. The solubility of nylon salt at 20°C, lower than the actual temperature of the salt solution, is equal to 0.480 g/L [21]. In order to produce this solubility, a water weight percent of about 72% in R-101 was used. A residence time of 30 minutes was assumed to be sufficient for a well-mixed outlet stream and a surge time of 10 minutes was assumed to be enough time for operators to respond to changes in process conditions. If the residence time is insufficient to produce well mixed conditions, the impeller speed inside the mixer can be increased to compensate.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined:

Installed Cost ($):	$1,050,000
Operating Cost ($/yr):	$1,320

The design calculation for R-101 is located on page A-47

The equipment specification sheet for R-101 is located on page 32

R-102

The volume of R-102, the CSTR that combines adipic acid and HMDA in the presence of deionized water in order to form nylon 6,6 salt, was calculated by using Equation 9.

The volumetric flowrate for the volume calculation of this reactor was set to be the outlet flowrate. This was done to avoid the ideal mixture assumption as the density of the salt solution could be more accurately calculated using Equations 10-12 [22].

$$\rho_w = 1.0046715 - (1.99824 * 10^{-4})T - (2.6321 * 10^{-6})T^2 \quad \textit{Equation 10}$$

$$\rho_{poly} = 1.13 - 0.00052 * T \quad \textit{Equation 11}$$

$$\rho_{soln} = (\frac{1}{\rho_w}\left(\omega_w + 0.925(1 - \omega_w - \omega_L)\right) + \left(\frac{1}{\rho_{poly}}\right)\omega_L)^{-1} \qquad \textit{Equation 12}$$

Where,

ρ_{soln} = the density of the nylon solution

ρ_w = the density of the water

ρ_{poly} = the density of the polymer

ω_w = the weight fraction of water in the solution

ω_L = the weight fraction of linkages in the solution

T = the temperature of the solution in degrees Celsius

The weight fraction of linkages was considered to be zero when calculating the density of the nylon 6,6 salt solution as the reactor temperature is not high enough for the polymerization reaction to occur.

The kinetics for the formation of the nylon 6,6 salt could not be found from a reputable source and therefore a residence time of 45 minutes was selected to match a patent found that included the same process [34]. A surge time of 5 minutes was determined to be enough time for operators to respond to a change in operating conditions. The assumption was made from this point forward in the process that the nylon 6,6 salt formation resulted in 100% conversion although in practice there would be some trace amounts of adipic acid and HMDA remaining the in the outlet stream.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$382,000
Operating Cost ($/yr):	$48,000

The design calculation for R-102 is located on page A-47

The equipment specification sheet for R-102 is located on page 33

R-103

The volume of R-103, the first CSTR in which the polymerization reaction occurs, was calculated using Equation 9. The volumetric flowrate was calculated using the conditions of the stream flowing out of the bottom of E-104, the falling-film evaporator, and applying Equations 10-12 in order to obtain the density of the solution entering the reactor. The residence time was assumed to be 3 hours, approximately one-fourth of the residence time of a batch reactor found in literature [15], and a surge time of 15 minutes was selected to allow operators time to respond to changes in operating conditions.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$670,000
Operating Cost ($/yr):	$801

The design calculation for R-103 is located on page A-47

The equipment specification sheet for R-103 is located on page 34

R-104

The volume of R-104, the second CSTR in which the polymerization reaction occurs, was calculated using Equation 9. The volumetric flowrate was obtained from the result of the Polymath simulations. The residence and surge times were set to the same values as those of R-103.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$536,000
Operating Cost ($/yr):	$753

The design calculation for R-104 is located on page A-48

The equipment specification sheet for R-104 is located on page 35

R-105

The volume of R-105, the third CSTR in which the polymerization reaction occurs, was calculated using Equation 9. The volumetric flowrate was obtained from the result of the Polymath simulations. The residence and surge times were set to the same values as those of R-103.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$519,000
Operating Cost ($/yr):	$740

The design calculation for R-105 is located on page A-48

The equipment specification sheet for R-105 is located on page 36

R-106

The volume of R-106, the fourth CSTR in which the polymerization reaction occurs, was calculated using Equation 9. The volumetric flowrate was obtained from the result of the Polymath simulations. The residence and surge times were set to the same values as those of R-103.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$514,000
Operating Cost ($/yr):	$731

The design calculation for R-106 is located on page A-48

The equipment specification sheet for R-106 is located on page 37

<u>R-107</u>

The volume of R-105, the fifth and final CSTR in which the polymerization reaction occurs, was calculated using Equation 9. The volumetric flowrate was obtained from the result of the Polymath simulations. The residence and surge times were set to the same values as those of R-103.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$511,000
Operating Cost ($/yr):	$730

The design calculation for R-107 is located on page A-49

The equipment specification sheet for R-107 is located on page 38

<u>V-101</u>

The volume of V-101, the holdup tank between R-102 and E-104, was calculated using Equation 13.

$$V = \frac{v_{0*} t_{holdup}}{\%_{normal\,fill}} \qquad \textit{Equation 13}$$

Where,

V = the volume of process vessel

v_0 = the volumetric flowrate into the process vessel

t_{holdup} = the holdup time of the process vessel

$\%_{normal\,fill}$ = the percent of total volume that is filled with liquid under normal operating conditions

The diameter of the vessel was then calculated by using Equation 14.

$$D = \left(\frac{V*4}{\frac{L}{D}*\pi}\right)^{1/3}$$ *Equation 14*

Where,
D = the diameter of the vessel
$\frac{L}{D}$ = the length to diameter ratio
V = the calculated volume of the vessel

The diameter was then rounded up to the nearest 3 inch interval. The actual volume of the vessel, based on the new diameter, was calculated using Equation 15.

$$V_{actual} = \left(\frac{\frac{L}{D}*\pi}{4}\right) * (D_{actual})^3$$ *Equation 15*

Where,

D_{actual} = the actual diameter of the vessel

$\frac{L}{D}$ = the length to diameter ratio
V_{actual} = the actual volume of the vessel

The volumetric flowrate was equal to the flowrate out of R-102. The holdup time was set to 5 minutes so that minor fluctuations in operating conditions do not stop the flow of nylon 6,6 salt solution throughout the process. The fraction of total volume filled with liquid under normal operation conditions was set to 50%.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$60,800
Operating Cost ($/yr):	N/A

The design calculation for V-101 is located on page A-49

The equipment specification sheet for V-101 is located on page 39

<u>V-102</u>

The volume of V-102, the condensate receiver for E-102, was determined using Equation 13. The same assumptions as were used for sizing V-101 aside from the flowrate which was obtained from Equation 10 using the conditions of the outlet of E-102. The diameter of the vessel was then calculated by using Equation 14, rounded up to the nearest 3 inches, and applied to Equation 15 to find the actual volume of V-102.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$39,200
Operating Cost ($/yr):	N/A

The design calculation for V-102 is located on page A-50

The equipment specification sheet for V-102 is located on page 40

E-101

The heat transfer area of E-101, the shell-and-tube heat-exchanger used to heat the deionized water stream entering R-101, was calculated using Equation 16.

$$A_0 = \frac{\dot{Q}}{U_o F \Delta T_{lm}} \quad \textit{Equation 16}$$

Where,

A_0 = the area of heat transfer

$\dot{Q}$ = the required heat transfer rate between the two streams inside the heat-exchanger

U_o = the overall heat transfer coefficient

F = the correction factor

ΔT_{lm} = the log mean temperature difference

The required heat transfer rate was calculated using the average specific heat of the deionized water inlet and outlet conditions and the mass flowrate of the water during startup conditions when there is no water recycle stream to lessen the load on the heat-exchanger. E-101 uses low pressure steam as its heat transfer fluid. The overall heat transfer coefficient and log-mean temperature are both calculated based on the properties of the product stream and low pressure steam. The correction factor is equal to 1 due to no temperature change in the low pressure steam.

Carbon steel was chosen as the material of construction due to its reduced cost, and the lack of corrosive materials in the process streams.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$127,000
Operating Cost ($/yr):	$48,800

The design calculation for E-101 is located on page A-53

The equipment specification sheet for E-101 is located on page 41

E-102

The heat transfer area of E-102, the shell-and-tube heat exchanger that acts as a condenser for the combined vent streams of the five polymerization reactors, was calculated using Equation 16. The required heat transfer rate was calculated to satisfy the demand of bringing the combined vent feed to 212°F and then condensing it. E-101 uses cooling water as its heat transfer fluid. The overall heat transfer coefficient and log mean temperature difference were calculated based on the properties of the product stream and cooling water. The correction factor was calculated based on the P and R values obtained from the temperature values of the heat-exchanger.

The feed into E-102 was considered to be pure steam although in practice there would be HMDA that is being vented as well. The simulation of the polymerization reaction assumes that no HMDA is being vented and therefore there isn't a calculated amount contained in the vent streams. In addition to this, the minute amounts of ammonium and carbon dioxide that are present in the vent stream were considered negligible for sizing purposes due to their extremely small concentrations.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$196,000
Operating Cost ($/yr):	$3,870

The design calculation for E-102 is located on page A-54

The equipment specification sheet for E-102 is located on page 42

<u>E-103</u>

The heat transfer area of E-103, the shell-and-tube heat exchanger that acts as a cooler for the outlet feed of V-102, was calculated using Equation 16. The required heat transfer rate was calculated based on heating the inlet stream to 140°F which matches the conditions of the deionized water entering R-101. E-103 uses cooling water as its heat transfer fluid. The overall heat transfer coefficient and log mean temperature difference were calculated based on the properties of the product stream and cooling water. The correction factor was calculated based on the P and R values obtained from the temperature values of the heat-exchanger.

The feed into E-103 was considered to be pure water, although in practice there would be some amount of HMDA that was vented out of the five polymerization reactors contained in the stream. The polymerization reaction simulation assumed no HMDA was being vented and therefore there is none calculated to be in the stream.

The material of construction was selected to be stainless steel in order to avoid equipment corrosion due to the basic nature of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$188,000
Operating Cost ($/yr):	$568

The design calculation for E-103 is located on page A-54

The equipment specification sheet for E-103 is located on page 43

E-104

The heat transfer area of E-104, the falling-film evaporator used to lower the weight percent of water in the nylon 6,6 salt stream, was calculated using Equation 17 [17].

$$A_0 = \frac{\dot{Q}}{U_0(T_{steam} - T_{bottoms})} \qquad \textit{Equation 17}$$

Where,

A_0 = the area of heat transfer

$\dot{Q}$ = the required heat transfer rate between the two streams inside the evaporator

U_o = the overall heat transfer coefficient

T_{steam} = the temperature of the steam being used at the heat transfer fluid

$T_{bottoms}$ = the temperature of the product stream

The required heat transfer rate was calculated using Equation 18 [4].

$$\dot{Q} = \dot{m}_{bottoms} h_{bottoms} + \dot{m}_{evap} h_{evap} - \dot{m}_{feed} h_{feed} \qquad \textit{Equation 18}$$

Where,

$\dot{Q}$ = the required heat transfer rate between the two streams inside the evaporator

$\dot{m}_{bottoms}$ = the mass flowrate of the product stream

$\dot{m}_{evap}$ = the mass flowrate of the water being evaporated out of the feed stream

$\dot{m}_{feed}$ = the mass flowrate of the feed stream entering the evaporator

$h_{bottoms}$ = the enthalpy of the product stream

h_{evap} = the enthalpy of the water being evaporated out of the feed stream

h_{feed} = the enthalpy of the feed stream entering the evaporator

The overall heat transfer coefficient was calculated as the average of typical values for a falling-film evaporator [17]. The temperature and weight percent of the bottom product stream was set to known values found in literature [18] in order to avoid surpassing the solubility limit of nylon 6,6 salt.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$427,000
Operating Cost ($/yr):	$850,000

The design calculation for E-104 is located on page A-55

The equipment specification sheet for E-104 is located on page 44

E-105

The heat transfer area of E-105, the shell-and-tube heat-exchanger that acts as a cooler for the nylon 6,6 melt leaving R-107, was calculated using Equation 16. E-105 uses cooling water as its heat transfer fluid and the overall heat transfer coefficient and log mean temperature difference were calculated based on the properties of the product stream and cooling water. The correction factor was calculated based on the P and R values obtained from the temperatures of the heat-exchanger.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$265,000
Operating Cost ($/yr):	$57

The design calculation for E-105 is located on page A-55

The equipment specification sheet for E-105 is located on page 45

P-101

The purchased horsepower of P-101, the pump that transfers the deionized water into R-101, was calculated by rounding up (to the nearest motor size) the result of Equation 19.

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$ *Equation 19*

Where,

bhp = the brake horsepower of the pump

$hyd\ hp$ = the hydraulic horsepower of the pump

ε_{pump} = the efficiency of the pump

The hydraulic horsepower of P-101 was calculated using Equation 20.

$$hyd\ hp = \frac{\Delta P * F}{1715}$$ *Equation 20*

Where,

$hyd\ hp$ = the hydraulic horsepower of the pump

ΔP = the pressure change generated by the pump in psi

F = the volumetric flowrate through the pump in gpm

The flowrate of the pump was calculated using the conditions of the deionized water feed and the pump efficiency was graphically estimated to be 0.35 based off of the flowrate [9]. This efficiency was applied across all pumps in the process as none have a high enough flowrate where this efficiency is not considered valid. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

The material of construction was selected to be carbon steel due to its lower price and the lack of contact with basic or acidic substances.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$30,600
Operating Cost ($/yr):	$496

The design calculation for P-101 is located on page A-57

The equipment specification sheet for P-101 is located on page 46

<u>P-102</u>

The purchased horsepower of P-102, the pump that transfers the aqueous HMDA solution from R-101 to R-102, was calculated by rounding up (to the nearest motor size) the result of Equation 19. The flowrate of the pump was calculated using the conditions of the outlet stream of R-101. The pump efficiency was confirmed to not graphically violate the value of 0.35 based off the flowrate [9]. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

The material of construction was selected to be stainless steel in order to avoid corrosion metals appearing the product stream due to the basic nature of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$42,200
Operating Cost ($/yr):	$496

The design calculation for P-102 is located on page A-57

The equipment specification sheet for P-102 is located on page 47

<u>P-103</u>

The purchased horsepower of P-103, the pump that transfers the nylon 6,6 salt solution from R-102 to V-101, was calculated by rounding up (to the nearest motor size) the result of Equation 19. The flowrate of the pump was calculated using the conditions of the outlet stream of R-102. The pump efficiency was confirmed to not graphically violate the value of 0.35 based off the flowrate [9]. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$42,300
Operating Cost ($/yr):	$380

The design calculation for P-103 is located on page A-57

The equipment specification sheet for P-103 is located on page 48

<u>P-104</u>

The purchased horsepower of P-104, the pump that transfers the nylon 6,6 salt solution from V-101 to E-104, was calculated by rounding up (to the nearest motor size) the result of Equation 19. The flowrate of the pump was calculated using the conditions of the outlet stream of V-101. The pump efficiency was confirmed to not graphically violate the value of 0.35 based off the flowrate [9]. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$44,000
Operating Cost ($/yr):	$951

The design calculation for P-104 is located on page A-58

The equipment specification sheet for P-104 is located on page 49

<u>P-105</u>

The purchased horsepower of P-105, the pump that transfers the nylon 6,6 salt solution from E-104 to R-103, was calculated by rounding up (to the nearest motor size) the result of Equation 19. The flowrate of the pump was calculated using the conditions of the outlet stream of E-104. The pump efficiency was confirmed to not graphically violate the value of 0.35 based off the flowrate [9]. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$74,700
Operating Cost ($/yr):	$2,260

The design calculation for P-105 is located on page A-58

The equipment specification sheet for P-105 is located on page 50

P-106

The purchased horsepower of P-106, the pump that transfers the nylon 6,6 melt from R-103 to R-104, was calculated by rounding up (to the nearest motor size) the result of Equation 19. The flowrate of the pump was obtained from the results of the Polymath simulation of the polymerization reaction. The pump efficiency was confirmed to not graphically violate the value of 0.35 based off the flowrate [9]. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$81,600
Operating Cost ($/yr):	$261

The design calculation for P-106 is located on page A-58

The equipment specification sheet for P-106 is located on page 51

P-107

The purchased horsepower of P-107, the pump that transfers the nylon 6,6 melt from R-104 to R-105, was calculated by rounding up (to the nearest motor size) the result of Equation 19. The flowrate of the pump was obtained from the results of the Polymath simulation of the polymerization reaction. The pump efficiency was confirmed to not graphically violate the value of 0.35 based off the flowrate [9]. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$43,600
Operating Cost ($/yr):	$261

The design calculation for P-107 is located on page A-59

The equipment specification sheet for P-107 is located on page 52

P-108

The purchased horsepower of P-108, the pump that transfers the nylon 6,6 melt from R-105 to R-106, was calculated by rounding up (to the nearest motor size) the result of Equation 19. The flowrate of the pump was obtained from the results of the Polymath simulation of the polymerization reaction. The pump efficiency was confirmed to not graphically violate the value of 0.35 based off the flowrate [9]. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$43,600
Operating Cost ($/yr):	$261

The design calculation for P-108 is located on page A-59

The equipment specification sheet for P-108 is located on page 53

P-109

The purchased horsepower of P-109, the pump that transfers the nylon 6,6 melt from R-106 to R-107, was calculated by rounding up (to the nearest motor size) the result of Equation 19. The flowrate of the pump was obtained from the results of the Polymath simulation of the polymerization reaction. The pump efficiency was confirmed to not graphically violate the value of 0.35 based off the flowrate [9]. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$43,600
Operating Cost ($/yr):	$261

The design calculation for P-109 is located on page A-59

The equipment specification sheet for P-109 is located on page 54

P-110

The purchased horsepower of P-110, the pump that transfers the water recycle stream from E-103 to R-101, was calculated by rounding up (to the nearest motor size) the result of Equation 19. The flowrate of the pump was calculated using the conditions of the outlet of V-102. The pump efficiency was confirmed to not graphically violate the value of 0.35 based off the flowrate [9]. The pressure change generated by the pump was calculated by subtracting the calculated suction pressure from the calculated discharge pressure based off of line losses and static head.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$43,200
Operating Cost ($/yr):	$261

The design calculation for P-110 is located on page A-60

The equipment specification sheet for P-110 is located on page 55

<u>X-101</u>

The required heat transfer rate generated by X-101, the furnace in which Duratherm is heated by natural gas, was calculated by Equation 21.

$$\dot{Q}_{furnace} = \sum \dot{Q}_{poly\ reactors}$$ *Equation 21*

Where,

$\dot{Q}_{furnace}$ = the heat transfer rate generated in the furnace

$\dot{Q}_{poly\ reactors}$ = the heat transfer rate generated in the polymerization reactors

The material of construction was selected to be carbon steel due to its lower price and the lack of contact with basic or acidic substances.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	2,190,000
Operating Cost ($/yr):	$281,000

The design calculation for X-101 is located on page A-61

<u>X-102</u>

The area of X-102, the apron conveyor belt transferring the adipic acid from X-104 into R-102, was calculated using Equation 22 [16].

$$A = \frac{F}{belt\ speed}$$ *Equation 22*

Where,

A = the area of the conveyor belt

F = the volumetric flowrate of the material being put onto the belt

$belt\ speed$ = the speed of the conveyor belt

The volumetric flowrate was calculated using the required mass flowrate of adipic acid and the density of adipic acid. The belt speed was selected to represent a slow, reasonable speed as to avoid powder being kicked up into the air.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$8,970
Operating Cost ($/yr):	N/A

The design calculation for X-102 is located on page A-61

The equipment specification sheet for X-102 is located on page 56

X-103

The area of X-103, the apron conveyor belt transporting the HMDA from X-105 to R-101, was calculated using Equation 22. The volumetric flowrate was calculated using the required mass flowrate of HMDA and the density of HMDA. The belt speed was selected to represent a slow, reasonable speed as to avoid powder being kicked up into the air.

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the alkalinity of HMDA.

Using cost correlations [31], the following costing information was determined.

Installed Cost ($):	$8,770
Operating Cost ($/yr):	N/A

The design calculation for X-103 is located on page A-62

The equipment specification sheet for X-103 is located on page 56

X-104

X-104, the hopper holding and dispensing adipic acid at a steady mass flowrate onto X-102, was determined to be comparable to an already existing product and was costed as such [29]. This hopper does not have a controllable mass disposable system and is therefore not a perfect comparison. In practice, the hopper would have a screw dispenser connected to a mass sensor in order to control a steady mass flowrate similar to one described in a patent [34].

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid.

Using direct cost quotes, the following costing information was determined.

Installed Cost ($):	$2,220
Operating Cost ($/yr):	N/A

The equipment specification sheet for X-104 is located on page 57

X-105

X-105, the hopper holding and dispensing HMDA at a controllable mass flowrate onto X-103, was determined to be comparable to an already existing product and was costed as such [29]. This hopper does not have a controllable mass disposable system and is therefore not a perfect comparison. In practice, the hopper would have a screw dispenser connected to a mass sensor in order to control a mass flowrate similar to one described in a patent [34].

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the alkalinity of HMDA.

Using direct cost quotes, the following costing information was determined.

Installed Cost ($):	$2,220
Operating Cost ($/yr):	N/A

The equipment specification sheet for X-105 is located on page 57

X-106

X-106 represents 122 separate yarn extruders and spinning machines that take the nylon 6,6 melt and spin it into sellable yarn. These extruders were determined to be comparable to an already existing product and priced as such [1].

Stainless steel was chosen as the material of construction in order to avoid corrosion in the equipment caused by the acidity of adipic acid and the alkalinity of HMDA.

Using direct cost quotes, the following costing information was determined.

Installed Cost ($):	$7,170,000
Operating Cost ($/yr):	$670,000

The equipment specification sheet for X-106 is located on page 58

Equipment Specification Sheets:

Table 9: R-101 Specification Sheet

Reactor				
Identification:	**Item** Item No. No. Required	Aqueous HMDA Mixer R-101 1		Date: 3/9/2017
Function: Mix the solid HMDA with water to make an aqueous solution				
Operation: Continuous				
Materials handled: Component Flow (lb/hr): Hexamethylene Diamine Water	 Stream 5 5245 0	 Stream 4 0 13300	 Stream 6 5245 13300	
Design Data: Temperature: Design Pressure: Material: Length: Diameter:	140°F 57.7 psig Stainless Steel 13.4 ft 4.5 ft			
Utilities: Electricity **Controls:** Level **Comments and Drawings:** See Process Flow Diagram and Appendix: A-47				

Table 10: R-102 Specification Sheet

Reactor				
Identification:	**Item**	Nylon Salt Reactor		
	Item No.	R-102		Date: 3/9/2017
	No. Required	1		
Function: Create the nylon 6,6 salt from adipic acid and HMDA				
Operation: Continuous				
Materials handled:				
Component Flow (lb/hr):	Stream 7	Stream 6	Stream 8	
Hexamethylene Diamine	0	5245	0	
Adipic Acid	6595	0	0	
Nylon 6,6 Salt	0	0	11840	
Water	0	13300	13300	
Design Data: Temperature:	140°F			
Design Pressure:	50 psig			
Material:	Stainless Steel			
Length:	15.6 ft			
Diameter:	5.25 ft			
Utilities: Low Pressure Steam, Electricity				
Controls: Level, Temperature				
Comments and Drawings: See Process Flow Diagram and Appendix: A-47				

Table 11: R-103 Specification Sheet

Reactor				
Identification:	**Item**	First Polymerization Reactor		
	Item No.	R-103		Date: 3/9/2017
	No. Required	1		
Function: Create Nylon 6,6 from its salt				
Operation: Continuous				
Materials handled:				
Component Flow (lb/hr):	Stream 12	Stream 19	Stream 13	
Nylon 6,6 Salt	11853	0	0	
Nylon 6,6	0	0	10547	
Water	5819	7124	0	
Ammonia	0	0.0207	0	
Carbon Dioxide	0	0.0268	0	
Design Data: Temperature:	622°F			
Design Pressure:	140.8 psig			
Material:	Stainless Steel			
Length:	22.2 ft			
Diameter:	7.4 ft			
Utilities: Hot Oil, Electricity				
Controls: Level, Temperature				
Comments and Drawings: See Process Flow Diagram and Appendix: A-47				

Table 12: R-104 Specification Sheet

Reactor				
Identification:	**Item**	Second Polymerization Reactor		Date: 3/9/2017
	Item No.	R-104		
	No. Required	1		
Function: Create Nylon 6,6 from its salt				
Operation: Continuous				
Materials handled:				
Component Flow (lb/hr):	Stream 13	Stream 20	Stream 14	
Nylon 6,6	10547	0	10364.11958	
Water	0	183.2	0	
Ammonia	0	0.0112	0	
Carbon Dioxide	0	0.0145	0	
Design Data: Temperature:	622°F			
Design Pressure:	138.9 psig			
Material:	Stainless Steel			
Length:	19.25 ft			
Diameter:	6.42 ft			
Utilities: Hot Oil, Electricity				
Controls: Level, Temperature				
Comments and Drawings: See Process Flow Diagram and Appendix: A-47				

Table 13: R-105 Specification Sheet

Reactor				
Identification:	**Item**	Third Polymerization Reactor		Date: 3/9/2017
	Item No.	R-105		
	No. Required	1		
Function: Create Nylon 6,6 from its salt				
Operation: Continuous				
Materials handled:				
Component Flow (lb/hr):	Stream 14	Stream 21	Stream 15	
Nylon 6,6	10364	0	10306	
Water	0	57.7	0	
Ammonia	0	0.0101	0	
Carbon Dioxide	0	0.0076	0	
Design Data: Temperature:	622°F			
Design Pressure:	139.1 psig			
Material:	Stainless Steel			
Length:	18.92 ft			
Diameter:	6.33 ft			
Utilities: Hot Oil, Electricity				
Controls: Level, Temperature				
Comments and Drawings: See Process Flow Diagram and Appendix: A-47				

Table 14: R-106 Specification Sheet

Reactor				
Identification:	**Item**	Fourth Polymerization Reactor		Date: 3/9/2017
	Item No.	R-106		
	No. Required	1		
Function: Create Nylon 6,6 from its salt				
Operation: Continuous				
Materials handled:				
Component Flow (lb/hr):	Stream 15	Stream 22	Stream 16	
Nylon 6,6	10306	0	10279	
Water	0	26.9	0	
Ammonia	0	0.0061	0	
Carbon Dioxide	0	0.0079	0	
Design Data: Temperature:	622°F			
Design Pressure:	139.1 psig			
Material:	Stainless Steel			
Length:	18.83 ft			
Diameter:	6.33 ft			
Utilities: Hot Oil, Electricity				
Controls: Level, Temperature				
Comments and Drawings: See Process Flow Diagram and Appendix:A-47				

Table 15: R-107 Specification Sheet

Reactor				
Identification:	**Item**	Fifth Polymerization Reactor		Date: 3/9/2017
	Item No.	R-107		
	No. Required	1		
Function: Create Nylon 6,6 from its salt				
Operation: Continuous				
Materials handled:				
Component Flow (lb/hr):	Stream 16	Stream 23	Stream 17	
Nylon 6,6	10279	0	10264	
Water	0	15.4	0	
Carbon Dioxide	0	0.0066	0	
Ammonia	0	0.0051	0	
Design Data: Temperature:	622°F			
Design Pressure:	139.1 psig			
Material:	Stainless Steel			
Length:	18.75 ft			
Diameter:	6.25 ft			
Utilities: Hot Oil, Electricity				
Controls: Level, Temperature				
Comments and Drawings: See Process Flow Diagram and Appendix: A-47				

Table 16: V-101 Specification Sheet

Vessel			
Identification:	**Item**	Nylon Salt Receiver	Date: 3/9/2017
	Item No.	V-101	
	No. Required	1	
Function: Hold nylon 6,6 salt exiting the Nylon salt reactor			
Operation: Continuous			
Materials handled:			
Component Flow (lb/hr):	Stream 8	Stream 9	
Nylon 6,6 Salt	25141	25141	
Design Data: Temperature:	140°F		
Design Pressure:	63.3 psig		
Material:	Stainless Steel		
Length:	9.75 ft		
Diameter:	3.25 ft		
Utilities:			
Controls: Level			
Comments and Drawings: See Process Flow Diagram and Appendix: A-49			

Table 17: V-102 Specification Sheet

Vessel			
Identification:	**Item**	Condensate Receiver	Date: 3/9/2017
	Item No.	V-102	
	No. Required	1	
Function: Hold water exiting the water recycle condenser and flash the carbon dioxide and ammonia			
Operation: Continuous			
Materials handled:			
Component Flow (lb/hr):	Stream 24	Stream 26	
Carbon Dioxide	0.0658	0.0658	
Ammonia	0.0508	0.0508	
Water	7393	7393	
Design Data: Temperature:	212°F		
Design Pressure:	70.7 psig		
Material:	Stainless Steel		
Length:	6.75 ft		
Diameter:	2.25 ft		
Utilities:			
Controls: Level			
Comments and Drawings: See Process Flow Diagram and Appendix: A-49			

Table 18: E-101 Specification Sheet

Heat Exchanger				
Identification:	**Item**	DI Water Heater		Date: 3/9/2017
	Item No.	E-101		
	No. Required	1		
Function: Heat the water feed to aid the dissolution of HMDA				
Operation: Continuous				
Materials handled:				
Component Flow (lb/hr):	Stream 2	Stream 3		
Water	5893	5893		
Design Data: TEMA Type:	AES			
Area:	29.04 ft^2			
Duty:	423838 BTU/hr			
Shell Temperature:	320 °F			
Shell Design Pressure:	90 psig			
Shell Phase:	Vapor			
Shell Material:	Stainless Steel			
Tube Temperature:	140 °F			
Tube Design Pressure:	70.7 psig			
Tube Phase:	Liquid			
Tube Material:	Stainless Steel			
Utilities: Low Pressure Steam				
Controls: Temperature				
Comments and Drawings: See Process Flow Diagram and Appendix: A-51				

Table 19: E-102 Specification Sheet

Heat Exchanger			
Identification:	**Item**	Water Recycle Condenser	Date: 3/9/2017
	Item No.	E-102	
	No. Required	1	
Function: Condense the water recycle stream			
Operation: Continuous			
Materials handled:			
Component Flow (lb/hr):	Stream 24	Stream 26	
Water	7408	7408	
Design Data: TEMA Type:	AES		
Area:	221.24 ft^2		
Duty:	8584070 BTU/hr		
Shell Temperature:	622 °F		
Shell Design Pressure:	122.5 psig		
Shell Phase:	Vapor		
Shell Material:	Stainless Steel		
Tube Temperature:	87 °F		
Tube Design Pressure:	100.0 psig		
Tube Phase:	Liquid		
Tube Material:	Stainless Steel		
Utilities: Cooling water			
Controls: Temperature			
Comments and Drawings: See Process Flow Diagram and Appendix: A-51			

Table 20: E-102 Specification Sheet

Heat Exchanger			
Identification:	**Item**	Water Recycle Cooler	
	Item No.	E-103	Date: 3/9/2017
	No. Required	1	
Function: Cool the water recycle stream			
Operation: Continuous			
Materials handled:			
Component Flow (lb/hr):	Stream 26	Stream 27	
Water	7408	7408	
Design Data: TEMA Type:	AES		
Area:	55.53 ft^2		
Duty:	534292 BTU/hr		
Shell Temperature:	87 °F		
Shell Design Pressure:	100.0 psig		
Shell Phase:	Liquid		
Shell Material:	Stainless Steel		
Tube Temperature:	212 °F		
Tube Design Pressure:	57.7 psig		
Tube Phase:	Liquid		
Tube Material:	Stainless Steel		
Utilities: Cooling water			
Controls: Temperature			
Comments and Drawings: See Process Flow Diagram and Appendix: A-51			

Table 21: E-103 Specification Sheet

Heat Exchanger				
Identification:	**Item**	Falling Film Evaporator		Date: 3/9/2017
	Item No.	E-104		
	No. Required	1		
Function: Evaporate some of the water from the salt reactor				
Operation: Continuous				
Materials handled:				
Component Flow (lb/hr):	Stream 9	Stream 10	Stream 11	
Water	13300	7469	5831	
Nylon 6,6 Salt	11841	0	11841	
Design Data: TEMA Type:	N/A			
Area:	83.98 ft^2			
Duty:	7322744 BTU/hr			
Operating Temperature:	320 °F			
Design Pressure:	90.0 psig			
Material:	Stainless Steel			
Utilities: Low Pressure Steam				
Controls: Temperature				
Comments and Drawings: See Process Flow Diagram and Appendix: A-51				

Table 22: E-105 Specification Sheet

Heat Exchanger			
Identification:	**Item**	Nylon 6,6 Melt Cooler	
	Item No.	E-105	Date: 3/9/2017
	No. Required	1	
Function: Cool the Nylon 6,6 melt			
Operation: Continuous			
Materials handled:			
Component Flow (lb/hr):	Stream 17	Stream 18	
Nylon 6,6	10264	10264	
Design Data: TEMA Type:	AES		
Area:	9.78 ft^2		
Duty:	438351 BTU/hr		
Shell Temperature:	87 °F		
Shell Design Pressure:	100.0 psig		
Shell Phase:	Liquid		
Shell Material:	Stainless Steel		
Tube Temperature:	622 °F		
Tube Design Pressure:	129.5 psig		
Tube Phase:	Liquid		
Tube Material:	Stainless Steel		
Utilities: Cooling water			
Controls: Temperature			
Comments and Drawings: See Process Flow Diagram and Appendix: A-51			

Table 23: P-101 Specification Sheet

Pump			
Identification:	**Item:**	DI Water Pump	Date:3/9/2017
	Item No.	P-101A/B	
	No. Required	2	
Function: Transport DI water to the DI water heater (E-101)			
Operation: Continuous			
Materials handled:			
Quantity (lbm/h):	Stream 1	Stream 2	
DI Water	5893	5893	
Design Data: Flow (gpm):	26.57		
Fluid Density (kg/L) :	0.99		
Discharge Pressure (psia):	35.40		
Delta P (psia):	20.40		
Shaft Power (Hp):	0.32		
Type:	Centrifugal		
Drive:	Electric		
Efficiency:	35%		
Motor Power (bhp):	1		
Motor Efficiency:	75%		
Purchased Power (hp):	1.33		
Material:	Stainless Steel		
Utilities: Electricity			
Controls:			
Comments and Drawings: See Process Flow Diagram and Appendix: A-55			

Table 24: P-102 Specification Sheet

Pump			
Identification:	**Item:**	Aqueous HMDA Pump	Date: 3/9/2017
	Item No.	P-102A/B	
	No. Required	2	
Function: Transport aqueous HMDA solution to the Nylon Salt Reactor (R-102)			
Operation: Continuous			
Materials handled:			
Quantity (lbm/h):	Stream 4	Stream 5	Stream 6
Solid HMDA	0	5245	5245
DI Water	13300	0	13300
Design Data: Flow (gpm):	39.29		
Fluid Density (kg/L) :	0.94		
Discharge Pressure (psia):	30.06		
Delta P (psia):	11.76		
Shaft Power (Hp):	0.27		
Type:	Centrifugal		
Drive:	Electric		
Efficiency:	35%		
Motor Power (bhp):	1		
Motor Efficiency:	75%		
Purchased Power (hp):	1.33		
Material:	Stainless Steel		
Utilities: Electricity			
Controls:			
Comments and Drawings: See Process Flow Diagram and Appendix: A-55			

Table 25: P-103 Specification Sheet

Pump			
Identification:	**Item:** Pump to Nylon Salt Receiver		Date:3/9/2017
	Item No. P-103A/B		
	No. Required 2		
Function: Transport nylon 6,6 salt from the nylon 6,6 salt reactor (R-102) to the nylon 6,6 salt receiver (V-101)			
Operation: Continuous			
Materials handled:			
Quantity (lbm/h):	Stream 6	Stream 7	Stream 8
Adipic Acid	0	6595	0
HMDA	5245	0	0
Water	13300	0	13300
Nylon 6,6 salt	0	0	25141
Design Data: Flow (gpm):	49.26		
Fluid Density (kg/L) :	1.02		
Discharge Pressure (psia):	28.00		
Delta P (psia):	7.62		
Shaft Power (Hp):	0.22		
Type:	Centrifugal		
Drive:	Electric		
Efficiency:	35%		
Motor Power (bhp):	0.75		
Motor Efficiency:	73.5%		
Purchased Power (hp):	1.02		
Material:	Stainless Steel		
Utilities: Electricity			
Controls:			
Comments and Drawings: See Process Flow Diagram and Appendix: A-55			

Table 26: P-104 Specification Sheet

	Pump		
Identification:	**Item:**	Pump to Evaporator	Date:3/9/2017
	Item No.	P-104A/B	
	No. Required	2	
Function: Transport nylon 6,6 salt from receiver (V-101) to thin film evaporator (E-104)			
Operation: Continuous			
Materials handled:			
Quantity (lbm/h):	Stream 8	Stream 9	
Nylon 6,6 salt	11840	11841	
Water	13300	13300	
Adipic Acid	0	0	
HMDA	0	0	
Design Data: Flow (gpm):	49.26		
Fluid Density (kg/L) :	1.02		
Discharge Pressure (psia):	35.30		
Delta P (psia):	18.95		
Shaft Power (Hp):	0.54		
Type:	Centrifugal		
Drive:	Electric		
Efficiency:	35%		
Motor Power (bhp):	2		
Motor Efficiency:	78.3%		
Purchased Power (hp):	2.55		
Material:	Stainless Steel		
Utilities: Electricity			
Controls:			
Comments and Drawings: See Process Flow Diagram and Appendix: A-55			

Table 27: P-105 Specification Sheet

Pump			
Identification:	**Item:**	Pump to Polymerization Reactor 1	Date: 3/9/2017
	Item No.	P-105A/B	
	No. Required	2	
Function: Transport nylon 6,6 salt solution from the thin film evaporator (E-104) to the first poly-reactor (R-103)			
Operation: Continuous			
Materials handled:			
Quantity (lbm/h):	Stream 11	Stream 12	
Nylon 6,6 Salt	11841	11853	
Water	5831	5819	
Design Data: Flow (gpm):	36.34		
Fluid Density (kg/L) :	0.97		
Discharge Pressure (psia):	105.54		
Delta P (psia):	80.29		
Shaft Power (Hp):	1.70		
Type:	Centrifugal		
Drive:	Electric		
Efficiency:	35%		
Motor Power (bhp):	5		
Motor Efficiency:	82.3%		
Purchased Power (hp):	6.07		
Material:	Stainless Steel		
Utilities: Electricty			
Controls:			
Comments and Drawings: See Process Flow Diagram and Appendix: A-55			

Table 28: P-106 Specification Sheet

Pump			
Identification:	**Item:**	Pump to Polymerization Reactor 2	Date: 3/9/2017
	Item No.	P-106A/B	
	No. Required	2	
Function:	Transport nylon 6,6 from Poly-Reactor 1 (R-103) to Poly-Reactor 2 (R-104)		
Operation:	Continuous		
Materials handled:			
Quantity (lbm/h):	Stream 12	Stream 13	
Nylon 6,6	0	10547	
Water	5819	0	
Nylon 6,6 Salt	11853	0	
Ammonia	0	0	
Carbon Dioxide	0	0	
Design Data:	Flow (gpm):	23.89	
	Fluid Density (kg/L) :	0.88	
	Discharge Pressure (psia):	103.60	
	Delta P (psia):	8.62	
	Shaft Power (Hp):	0.12	
	Type:	Centrifugal	
	Drive:	Electric	
	Efficiency:	35%	
	Motor Power (bhp):	0.50	
	Motor Efficiency:	71.4%	
	Purchased Power (hp):	0.70	
	Material:	Stainless Steel	
Utilities:	Electricity		
Controls:			
Comments and Drawings:	See Process Flow Diagram and Appendix: A-55		

Table 29: P-107 Specification Sheet

Pump			
Identification:	**Item:**	Pump to Polymerization Reactor 3	Date: 3/9/2017
	Item No.	P-107A/B	
	No. Required	1	
Function: Transport nylon 6,6 from Poly-Reactor 2 (R-104) to Poly-Reactor 3 (R-105)			
Operation: Continuous			
Materials handled:			
Quantity (lbm/h):	Stream 13	Stream 14	
Nylon 6,6	10547	10364	
Water	0	0	
Design Data: Flow (gpm):	22.46		
Fluid Density (kg/L) :	0.92		
Discharge Pressure (psia):	103.75		
Delta P (psia):	9.55		
Shaft Power (Hp):	0.12		
Type:	Centrifugal		
Drive:	Electric		
Efficiency:	35%		
Motor Power (bhp):	0.5		
Motor Efficiency:	71.4%		
Purchased Power (hp):	0.70		
Material:	Stainless Steel		
Utilities: Electricity			
Controls:			
Comments and Drawings: See Process Flow Diagram and Appendix: A-55			

Table 30: P-108 Specification Sheet

Pump			
Identification:	**Item:**	Pump to Polymerization Reactor 4	Date: 3/9/2017
	Item No.	P-108A/B	
	No. Required	1	
Function:	Transport nylon 6,6 from Poly-Reactor 3 (R-105) to Poly-Reactor 4 (R-106)		
Operation:	Continuous		
Materials handled:			
Quantity (lbm/h):	Stream 14	Stream 15	
Nylon 6,6	10364	10306	
Water	0	0	
Design Data:	Flow (gpm):	22.09	
	Fluid Density (kg/L) :	0.93	
	Discharge Pressure (psia):	103.81	
	Delta P (psia):	9.66	
	Shaft Power (Hp):	0.12	
	Type:	Centrifugal	
	Drive:	Electric	
	Efficiency:	35%	
	Motor Power (bhp):	0.36	
	Motor Efficiency:	71.4%	
	Purchased Power (hp):	0.70	
	Material:	Stainless Steel	
Utilities: Electricity			
Controls:			
Comments and Drawings: See Process Flow Diagram and Appendix: A-55			

Table 31: P-109 Specification Sheet

Pump			
Identification:	**Item:**	Pump to Polymerization Reactor 5	Date: 3/9/2017
	Item No.	P-109A/B	
	No. Required	1	
Function:	Transport nylon 6,6 from Poly-Reactor 4 (R-106) to Poly-Reactor 5 (R-107)		
Operation:	Continuous		
Materials handled:			
Quantity (lbm/h):	Stream 15	Stream 16	
Nylon 6,6	10306	10279	
Water	0	0	
Design Data:	Flow (gpm):	21.80	
	Fluid Density (kg/L) :	0.94	
	Discharge Pressure (psia):	103.83	
	Delta P (psia):	9.67	
	Shaft Power (Hp):	0.12	
	Type:	Centrifugal	
	Drive:	Electric	
	Efficiency:	35%	
	Motor Power (bhp):	0.5	
	Motor Efficiency:	71.4%	
	Purchased Power (hp):	0.70	
	Material:	Stainless Steel	
Utilities:	Electricity		
Controls:			
Comments and Drawings:	See Process Flow Diagram and Appendix: A-55		

Table 32: P-110 Specification Sheet

	Pump		
Identification:	**Item:**	Water Recycle Pump	Date: 3/9/2017
	Item No.	P-110A/B	
	No. Required	1	
Function:	Transports liquid condensate from V-102 to the water recycle cooler (E-103)		
Operation:	Continuous		
Materials handled:			
Quantity (lbm/h):	Stream 24	Stream 26	
Water	7408	7408	
Design Data:	Flow (gpm):	15.44	
	Fluid Density (kg/L) :	0.96	
	Discharge Pressure (psia):	35.40	
	Delta P (psia):	18.40	
	Shaft Power (Hp):	0.17	
	Type:	Centrifugal	
	Drive:	Electric	
	Efficiency:	35%	
	Motor Power (bhp):	0.5	
	Motor Efficiency:	71.4%	
	Purchased Power (hp):	0.70	
	Material:	Stainless Steel	
Utilities:	Electricity		
Controls:			
Comments and Drawings:	See Process Flow Diagram and Appendix: A-55		

Table 33: X-102 Specification Sheet

Conveyor			
Identification:	**Item**	Adipic Acid Conveyor	Date: 3/9/2017
	Item No.	X-102	
	No. Required	1	
Function: Transport the adipic acid from its hopper to the salt reactor			
Operation: Continuous			
Materials handled:			
Component Flow (lb/hr):	Stream 7		
Adipic Acid	6595		
Design Data: Belt Area:	0.125522 ft^2		
Belt Velocity:	492.126 ft/hr		
Utilities: Electricity (negligible)			
Controls:			
Comments and Drawings: See Process Flow Diagram and Appendix: A-61			

Table 34: X-103 Specification Sheet

Conveyor			
Identification:	**Item**	HMDA Conveyor	Date: 3/9/2017
	Item No.	X-103	
	No. Required	1	
Function: Transport the HMDA from its hopper to the HMDA mixer			
Operation: Continuous			
Materials handled:			
Component Flow (lb/hr):	Stream 5		
Hexamethylene Diamine	5245		
Design Data: Belt Area:	0.203226 ft^2		
Belt Velocity:	492.126 ft/hr		
Utilities: Electricity (negligible)			
Controls:			
Comments and Drawings: See Process Flow Diagram and Appendix: A-61			

Table 35: X-104 Specification Sheet

Hopper			
Identification:	**Item**	Adipic Acid Hopper	Date: 3/9/2017
	Item No.	X-104	
	No. Required	1	
Function: Hold nylon 6,6 salt exiting the Nylon salt reactor			
Operation: Continuous			
Materials handled:			
Component Flow (lb/hr):	Stream 7		
Adipic Acid	6595		
Design Data: Volume:	6.831 ft^3		
Material:	Stainless Steel		
Utilities:			
Controls: Flowrate			
Comments and Drawings: See Process Flow Diagram			

Table 36: X-105 Specification Sheet

Hopper			
Identification:	**Item**	HMDA Hopper	Date: 3/9/2017
	Item No.	X-105	
	No. Required	1	
Function: Hold nylon 6,6 salt exiting the Nylon salt reactor			
Operation: Continuous			
Materials handled:			
Component Flow (lb/hr):	Stream 5		
Hexamethylene Diamine	5245		
Design Data: Volume:	6.831 ft^3		
Material:	Stainless Steel		
Utilities:			
Controls: Flowrate			
Comments and Drawings: See Process Flow Diagram			

Table 37: X-106 Specification Sheet

Extruder				
Identification:	**Item**	Yarn Extruder		
	Item No.	X-106	Date: 3/9/2017	
	No. Required	122		
Function: Hold nylon 6,6 salt exiting the Nylon salt reactor				
Operation: Continuous				
Materials handled:				
Component Flow (lb/hr):	Stream 18			
Nylon 6,6	10264			
Design Data: Capacity:	84.13 lb/hr			
Material:	Stainless Steel			
Utilities: Electricity				
Controls:				
Comments and Drawings: See Process Flow Diagram				

Equipment Cost Summary:

Table 38: Equipment Bare Module Costs

Equipment #	Purchase Price	Quantity	Total Purchase Price	Price Source
R-101	$622,000	1	$622,000	Cost Correlation
R-102	$227,000	1	$227,000	Cost Correlation
R-103	$399,000	1	$399,000	Cost Correlation
R-104	$319,000	1	$319,000	Cost Correlation
R-105	$309,000	1	$309,000	Cost Correlation
R-106	$306,000	1	$306,000	Cost Correlation
R-107	$304,000	1	$304,000	Cost Correlation
V-101	$42,800	1	$42,800	Cost Correlation
V-102	$27,600	1	$27,600	Cost Correlation
E-101	$75,600	1	$75,600	Cost Correlation
E-102	$136,000	1	$136,000	Cost Correlation
E-103	$129,000	1	$129,000	Cost Correlation
E-104	$254,000	1	$254,000	Cost Correlation
E-105	$183,000	1	$183,000	Cost Correlation
P-101	$10,700	2	$21,400	Cost Correlation
P-102	$15,600	2	$31,200	Cost Correlation
P-103	$15,600	2	$31,200	Cost Correlation
P-104	$16,300	2	$32,600	Cost Correlation
P-105	$19,300	2	$38,600	Cost Correlation
P-106	$16,100	2	$32,200	Cost Correlation
P-107	$16,100	2	$32,200	Cost Correlation
P-108	$16,100	2	$32,200	Cost Correlation
P-109	$16,100	2	$32,200	Cost Correlation
P-110	$16,000	2	$32,000	Cost Correlation
X-101	$1,300,000	1	$1,300,000	Cost Correlation
X-102	$5,340	1	$5,340	Cost Correlation
X-103	$5,220	1	$5,220	Cost Correlation
X-104	$1,320	1	$1,320	Quotation [29]
X-105	$1,320	1	$1,320	Quotation [29]
X-106	$35,000	122	$4,270,000	Quotation [1]

Fixed Capital Investment Summary:

The fixed capital investment value of each piece of equipment was found by calculating the total grass-roots installed cost using Equations 23 and 24.

$$C_{TM} = 1.18 \sum C_{BM} \quad \textit{Equation 23}$$

$$C_{GR} = C_{TM} + 0.5 \sum C_{BM}^{\circ} \quad \textit{Equation 24}$$

Where,

C_{TM} = the total module cost of the piece of equipment

C_{BM} = the bare module cost, or purchase price, of the piece of equipment

C_{GR} = the grass-roots installed cost of the piece of equipment

C_{BM}° = the bare module cost of base conditions of the piece of equipment

The results of applying these equations to all process equipment are summarized in Table 39.

Table 39: Equipment Total Module Costs

Equipment #	Purchase Price	Quantity	Total Installed Cost
R-101	$622,000	1	$1,050,000
R-102	$227,000	1	$382,000
R-103	$399,000	1	$670,000
R-104	$319,000	1	$536,000
R-105	$309,000	1	$519,000
R-106	$306,000	1	$514,000
R-107	$304,000	1	$511,000
V-101	$42,800	1	$60,800
V-102	$27,600	1	$39,200
E-101	$75,600	1	$127,000
E-102	$136,000	1	$196,000
E-103	$129,000	1	$188,000
E-104	$254,000	1	$427,000
E-105	$183,000	1	$265,000
P-101	$10,700	2	$30,600
P-102	$15,600	2	$42,200
P-103	$15,600	2	$42,300
P-104	$16,300	2	$44,000
P-105	$19,300	2	$74,700
P-106	$16,100	2	$81,600
P-107	$16,100	2	$43,600
P-108	$16,100	2	$43,600
P-109	$16,100	2	$43,600
P-110	$16,000	2	$43,200
X-101	$1,300,000	1	$2,190,000
X-102	$5,340	1	$8,970

X-103	$5,220	1	$8,770
X-104	$1,320	1	$2,220
X-105	$1,320	1	$2,220
X-106	$35,000	122	$7,170,000

Safety, Health, and Environmental Considerations:

Safety Considerations:

Safety is the top priority when running a process. When designing a process there are four major factors that affect safety. These are high operating pressures, temperatures, highly reactive components, and exposed equipment. These concerns are addresses in the design by choosing the appropriate material of construction, taking into account pressure factors in the equipment design, safeguards for exposed equipment, and the control strategy. The determination of the materials of construction depended on whether the equipment was exposed to corrosive material; if it was then stainless steel was chosen, otherwise carbon steel was used. All process equipment will be designed to withstand pressures 50 psi above normal operating conditions. Pressurized vessels will be designed with thicker walls than necessary for safety reasons. Extruders with moving machinery are required for this process so operating procedures should be design with this in mind to prevent workplace accidents. The process design pressure and temperature will be set by the process control strategy. Using pressure, level, temperature, and flow controllers the process streams will be kept within the optimal ranges for production and safety.

Identifying hazards is key to designing a safe process. A What-If-Analysis was performed for the whole process. Items that were considered but were not found to be concern were runaway reactions, fire hazards, explosions, and alternative reaction chemistry. Runaway reactions were found to not be a concern since the heat of reaction for the process is vastly smaller than that of the heat of vaporization of water. So the feed is being cooled down faster than the reaction is occurring. Fire hazards were found not to be a concern due to all the temperatures within the process being below the flammability limit of the chemicals. Explosions were also found not to be a concern for the same reason as fire hazards. A Process Hazard Analysis (PHA) was performed on the hazards that were a safety concern to the process. These hazards are tabulated in Table 40. The hazards are categorized as Negligible (I), Marginal (II), Critical (III), Catastrophic (IV).

Table 40: Process Hazard Analysis

Hazard	Cause	Major Effects	Hazard Category	Corrective/Preventative Measure
Toxic Release	1) HMDA pipe leak	Release of chemicals into the environment	I	(a) Provide a leak detection system (b) Implement procedure for pipeline inspection
	2) HMDA particulates escaping the hopper	Potential minor injuries	II	(a) Operators have proper PPE (Personal Protective Equipment) (b) Enclose the hopper
	3) Adipic Acid Exposure	Release of chemicals into the environment and potential minor injuries	II	(a) Proper PPE for handling
Mechanical Hazard	1) Moving machinery	Potential injuries	III	(a) Operating procedures to prevent workplace accidents
Elevated Temperature	1) Hot material release 2) Contact with hot surface	Potential minor injuries	II	(a) Labels that indicate a hot hazard (b) Insulation on the pipes
Combustibility	1) Dust Explosion	Potential injuries and death	IV	(a) Making HMDA aqueous by adding water (b) Make the hopper and conveyor system more enclosed
Runaway Reactions	1) Uncontrolled polymerization	Release of chemical into the environment	I	(a) Control valves to shut off the feed

An inherent safety approach was applied to the hazards in order to determine ways to make the process inherently safer. These action items are tabulated in Table 41.

Table 41: Inherent Safety Measures

Hazard	Inherent Safety Concept	Action
Toxicity from dry HMDA	Attenuation	Made aqueous HMDA early in the process
Containment	Intensification	Maximized concentration of adipic acid and HMDA based on solubility
Reactor rupture	Attenuation	Minimizing pressure in R-(102-107)
Overly complex design	Simplification	Restricted the number of CSTRs to five

Health Considerations:

Both the chemicals used in the process and the by-products created during the process present safety concerns. The reactants that pose a safety concern are adipic acid and hexamethylene diamine (HMDA). The main by-product that poses a safety concern is ammonia.

Adipic Acid is a white crystalline solid. The dust from this crystalline solid is combustible, so appropriate exhaust ventilation is required. Adipic Acid must be stored in a tightly closed container in a dry and well ventilated area. Exposure hazards to this chemical include severe eye irritation when in contact with eyes. Proper personal protective equipment (PPE) for handling adipic acid include safety glasses, gloves, impervious clothing, and respiratory protection from the dust particles. Adipic Acid decomposes into hazardous carbon oxides under fire conditions [23].

Hexamethylene diamine is a colorless, odorless, corrosive solid. Exposure hazards to this chemical include being an oral toxin if ingested and cause respiratory irritation. Any skin or eye contact can lead to severe skin burns and serious eye damage. To limit the dust exposure to operators, HMDA will be mixed with water making it an aqueous solution before entering the mixer with the adipic acid. PPE for handling HMDA include face shield, safety glasses, gloves, complete body suit, and air-purifying respirators. HMDA must be stored under inert gas in a tightly closed container in a dry and well-ventilated place. HMDA decomposes into hazardous carbon oxides and nitrogen oxides under fire conditions. [24]

Carbon Dioxide is a colorless and odorless gas. Exposure hazards to this chemical include asphyxiation, dizziness, drowsiness, increased heart rate, and nervous system damage. Carbon dioxide decomposes into carbon monoxide and oxygen under high temperatures. [19]

Ammonia is a colorless, flammable compressed gas. Exposure hazards to this chemical include acute toxicity if inhaled, skin corrosion and serious eye damage if contact with skin and eyes. PPE for handling ammonia include safety goggles, face shield, gloves, complete body suit, and air-purifying respirators. Keep away from sources of ignition and take measures to prevent the buildup of electrostatic charge. Ammonia decomposes into hazardous nitrogen oxides under fire conditions. [25]

Environmental Considerations:

All chemicals are considered hazardous waste and need to undergo waste treatment as per OSHA regulations before being released into the environment. The waste water collected from E-104 will be shipped to an external source where the water will be treated. The inert gases, which consist of carbon dioxide and ammonia, collected from V-102 will be sent to a scrubber unit and then released to the atmosphere.

Calvert City requires several permits in order to construct a manufacturing facility within its city limits. These permits include: Land Use Permit, Development Permit, Alarm Permit, and a Fire Systems Permit/Inspection. A land use permit needs to be obtained in order to occupy and develop public land. A development permit works in tangent with the Land Use Permit in order to construct the manufacturing facility and allow for proper drainage modifications. An alarm system will be operated at the facility so an alarm permit will need to be obtained before the alarm system can be used. The manufacturing facility will be working with flammable chemicals so a fire alarm permit is required for the construction of the fire suppression system [3].

After the construction of the facility, process safety management should be further investigated. OSHA 1910.119 has permit requirements for practices and procedures to protect employees. A system will need to be set up to issue permits for confined space, which is required to perform any maintenance work inside the polymerization reactors and mixer. A system will also need to be set up for hot work permits whenever any work that produces a source of ignition occurs due to the flammability of the chemicals used.

Other Important Considerations:

Startup:

The startup procedure for the plant will involve turning on the feed lines to the system; the adipic acid and HMDA will be dispensed from their hoppers at the steady state rates initially, but the water flow being mixed with the HMDA will need to be larger than the steady state rate since the recycle stream is not operational at this point. Once the feeds are online, the salt CSTR will be heated up to its reaction temperature by opening the LPS line into the jacket. The feeds will then flow into the CSTR and begin accumulating and reacting. Once the liquid level in the reactor reaches the desired steady state value, the liquid outlet will be opened, allowing the stream to proceed into the liquid holdup tank. Once the liquid in the tank reaches the desired level, the outlet stream will be opened. The hot oil stream will then begin entering the jacket of the first polymerization CSTR, getting the reactor to the required reaction temperature. The CSTR will begin filling up, when the liquid reaches the desired level the liquid outlet, as well as the gas vent, will both be opened. This will start the recycle steam, so the inlet water flowrate will need to be adjusted down to compensate. This process will be repeated for the next four polymerization CSTRs. After the fifth CSTR outlet is opened, the product stream will need to be monitored to determine when steady state is reached and thus when product meeting the specification is produced. Once steady state is achieved, normal operating conditions are maintained. During startup, until steady state is achieved, a significant loss of revenue will occur since the product being produced is not sellable until it reaches the desired specification. . The yarn extruder will also require threading during start up. During shutdown, the polymer melt should be drained from the system to prevent unnecessary fouling and clogging of the equipment.

Control Strategy:

Table 42 summarizes the variables that are manipulated and controlled during the normal operation on this process. It also lists the actuators and sensors required for the outlined control strategy.

Table 42: Process Control Scheme

Location	Manipulated Variable	Control Variable	Actuator	Sensor
Solid Stream 5	Screw Extruder Speed	R-101 HMDA Concentration	Screw Extruder	Mass Flow Sensor
Solid Stream 7	Screw Extruder Speed	Stream 7 Mass Flowrate	Screw Extruder	Concentration Sensor
Stream 3	Stream 3 Flowrate	Stream 3 Flowrate	Control Valve	Flow Sensor
E-101	Low Pressure Steam Flowrate	Stream 3 Temperature	Control Valve	Temperature Sensor
R-101 through R-107	Liquid flowrate leaving the reactor	Reactor Liquid Level	Control Valve	Liquid Level Sensor
R-102	LPS flowrate through R-101 jacket	Stream 8 Temperature	Control Valve	Temperature Sensor
V-101 and V-102	Liquid flowrate leaving the vessel	Vessel Liquid Level	Control Valve	Liquid Level Sensor
E-104	Low Pressure Steam Flowrate	E-104 Temperature	Control Valve	Temperature Sensor
Stream 8	Liquid flowrate leaving E-104	E-104 Liquid Level	Control Valve	Liquid Level Sensor
R-103 through R-107	Vapor flowrate leaving the reactor	Reactor Pressure	Control Valve	Pressure Sensor
R-103 through R-107	Hot Oil Flowrate	Reactor Temperature	Control Valve	Temperature Sensor
E-103 and E-105	Cooling Water Flowrate	Outlet Process Stream Temperature	Control Valve	Temperature Sensor
E-102	Cooling Water Flowrate	Stream 24 Pressure	Control Valve	Pressure Sensor
V-102	Stream 25 Flowrate	V-102 Pressure	Control Valve	Pressure Sensor

The control strategy requires the concentration of HMDA in R-101 to be monitored to control the addition of solid HMDA. This feedback loop is required for HMDA and not adipic acid due to the relatively high volatility of HMDA with respect to adipic acid. Although it was assumed that no HMDA was vented from the polymerization reactors, the recycle stream will contain some amount of HMDA during operation [18]. The concentration feedback loop should be able to maintain the equimolar feed ratio of HMDA and adipic acid during operation and prevent the vented HMDA from going to waste.

Attempts were made to minimize the pressure where possible. Controlling the pressure of the reactor vents may present some problems. The control strategy calls for the vent pressures to be controlled by the rate of condensation, which is in turn controlled by the flowrate of the cooling water through E-102. If this proves insufficient, the pressure in the polymerization reactors will rise to match the pressure of the vent system as their pressure is controlled by the flowrate of the vapor leaving the reactors. Pressure relief systems mitigate the risk of a containment breach and if operating pressure is unable to be maintained a larger condenser or another condenser in series with the designed condenser would be required.

Using a series of CSTRs allows for a greater degree of pressure control as each reactor is able to double as a vapor-liquid separator. The use of centrifugal pumps results in the majority of the control being done with control valves which are well understood actuators. The only actuators that are not control valves are those that deal with solid reactants.

R-101	R-102	R-103	R-104	R-105	R-106	R-107	V-101	V-102	E-101	E-102	E-103
Aqueous HDMA Mixer	Nylon Salt Reactor	First Poly. Reactor	Second Poly. Reactor	Third Poly. Reactor	Fourth Poly. Reactor	Fifth Poly. Reactor	Nylon Salt Receiver	Condensate Receiver	DI Water Heater	Water Recycle Condenser	Water Recycle Cooler

E-104	E-105	P-101	P-102	P-103	P-104	P-105	P-106	P-107	P-108	P-109	P-110	P-111
Falling Film Evaporator	Nylon 6,6 Melt Cooler	DI Water Pump	Aqueous HDMA pump	Pump to Nylon Salt Receiver	Pump to Evaporator	First Pump to Poly. Reactor 1	Second Pump to Poly. Reactor 1	Third Pump to Poly. Reactor 1	Fourth Pump to Poly. Reactor 1	Fifth Pump to Poly. Reactor 1	Pump to Poly. Reactor 3	Pump to Poly. Reactor 4

P-112	P-113	P-114	X-101	X-102	X-103	X-104	X-105	X-106	X-107
Pump to Poly. Reactor 5	Pump to Nylon 6,6 Melt Cooler	Water Recycle Pump	Hot Oil Furnace	Adipic Acid Conveyor	HDMA Conveyor	Solid Adipic Acid Hopper	Solid HDMA Hopper	Granule Extruders	Yarn Extruders

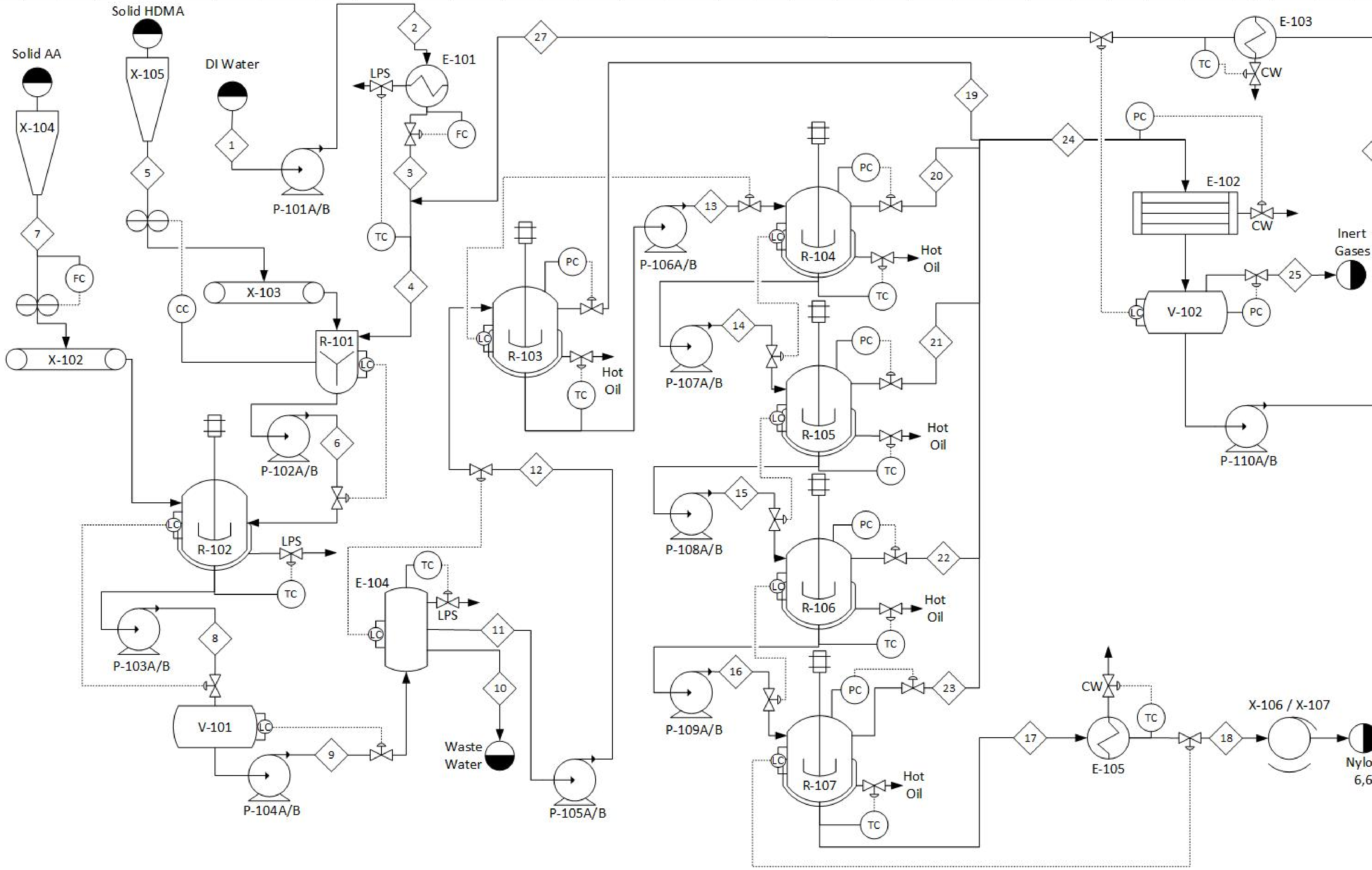

Figure 3: Control Strategy PFD

Manufacturing Costs (exclusive of Capital Requirements):

Table 43 is analogous to Table 8.2 in Turton and was used to calculate the cost of manufacturing (COMd) [31]. The calculated COMd does not include the term for depreciation as MACRS depreciation, a more rigorous method of calculating depreciation, is used in its place.
Since this design is for a grassroots facility, none of the other factors could be neglected and so the midpoint of each of the typical range of multiplying factors was used. Of particular note are the lines that estimate the cost of patents and royalties and research and development. A patent for a process similar to the one used for the nylon 6,6 salt production featured heavily in the design of this process which would likely justify the admittedly high cost of this line item. Similarly, many of the recommendations and assumptions included in this report will require extensive research to implement and verify which justifies the expense of research and development.

The annual cost of waste treatment (CWT) and the annual cost of utilities (CUT) were both calculated using the mass and energy balances found in the appendix and Table 8.3 of Turton [31]. A summary of the cost of the individual utilities and waste treatment can be found in Table 7. The cost of waste treatment is essentially negligible as it represents less than 0.1% of the COMd. The CWT is only taking the water removed from the falling film evaporator into account due to the negligible flowrate, 0.12 lbm/hr, of the inert gases.

The number of required operators per shift was calculated based on the number of pieces of process equipment, excluding pumps and process vessels, and the number of processing steps involving the handling of particulate solids. The total number of required operators was estimated to be 4.5 times greater than the number of operators that were required per shift. The number of operators when combined with the annual mean wage of chemical plant and system operators in the West Kentucky nonmetropolitan area, $63,920, was used to calculate the annual cost of operator labor (COL) in the appendix.

The annual cost of raw materials (CRM) is the single largest contributor to the COMd of this process, as can be seen in Table 44. The CRM was calculated using mass flowrates that would provide the required 85 million pounds of nylon 6,6 per year, the prices for adipic acid and HMDA quoted from Invista [13], and the price of deionized water found in Turton [31]. The fixed capital investment (FCI) is summarized in Table 39.

Table 43: Cost of Manufacturing Factors

1	**Direct Manufacturing Costs**	Typical Range of Multiplying Factors	Value Used in Design
a	Raw Materials	CRM	CRM
b	Waste Treatment	CWT	CWT
c	Utilities	CUT	CUT
d	Operating Labor	COL	COL
e	Direct Supervisory and Clerical Labor	(0.1-0.25)COL	0.18COL
f	Maintenance and Repairs	(0.02-0.1)FCI	0.06FCI
g	Operating Supplies	(0.1-0.2)(Line 1.F)	0.009FCI
h	Laboratory Charges	(0.1-0.2)COL	0.15COL
i	Patents and Royalties	(0-0.06)COM	0.03COM

Total Direct Manufacturing Costs		CRM+CWT+CUT+1.33COL+0.03COM+0.069FCI	
2	**Fixed Manufacturing Costs**	Typical Range of Multiplying Factors	Value Used in Design
a	Depreciation	0.1FCI	*0
b	Local Taxes and Insurance	(0.014-0.05)FCI	0.032FCI
c	Plant Overhead Costs	(0.50-0.7)(Line 1.D + Line 1.E + Line 1.F)	0.708COL+0.036FCI
Total Fixed Manufacturing Costs		0.708COL+0.068FCI	
3	**General Manufacturing Expenses**	Typical Range of Multiplying Factors	Value Used in Design
a	Administration Costs	(0.50-0.7)(Line 1.D + Line 1.E + Line 1.F)	0.177COL+0.009FCI
b	Distribution and Selling Costs	(0.02-0.2)COM	0.11COM
c	Research and Development	0.05COM	0.05COM
Total General Manufacturing Costs		0.177COL+0.009FCI+0.16COM	
Total Costs		CRM+CWT+CUT+2.215COL+0.16COM+0.146FCI	
COMd		0.180FCI+2.73COL+1.23(CRM+CWT+CUT)	

Table 44: Manufacturing Costs for Granule Case

CRM	Annual Cost of Raw Materials	$ 91,500,000
CWT	Annual Cost of Waste Treatment	$ 1,160
CUT	Annual Cost of Utilities	$ 1,290,000
COL	Annual Cost of Operator Labor	$ 3,390,000
FCI	Annual Fixed Capital Investment	$ 8,650,000
COMd	Annual Cost of Manufacturing	$ 125,000,000
	Cost of Manufacturing per lbm Nylon 66	$ 1.48

Table 45: Manufacturing Costs for Fiber Case

CRM	Annual Cost of Raw Materials	$ 91,500,000
CWT	Annual Cost of Waste Treatment	$ 1,160
CUT	Annual Cost of Utilities	$ 1,910,000
COL	Annual Cost of Operator Labor	$ 3,710,000
FCI	Annual Fixed Capital Investment	$ 15,350,000
COMd	Annual Cost of Manufacturing	$ 128,000,000
	Cost of Manufacturing per lbm Nylon 66	$ 1.51

It is readily apparent that the fiber case will be the preferred design as granular nylon costs significantly more to produce, $1.51, than it can be sold for, $0.76. Even if this were not the case, the COMd for nylon fiber is less than 3% more expensive. Tables 44 and 45 compare the nylon fiber and granular nylon case and it is clear that only the fiber case warrants further investigation in the form of the turndown case and the sensitivity analysis.

Table 46: Manufacturing Costs for Turndown Fiber Case

				% of full production case
CRM	Annual Cost of Raw Materials	$	1,300,000	67%
CWT	Annual Cost of Waste Treatment	$	770	67%
CUT	Annual Cost of Utilities	$	1,500,000	79%
COL	Annual Cost of Operator Labor	$	3,710,000	100%
FCI	Annual Fixed Capital Investment	$	15,350,000	100%
COMd	Annual Cost of Manufacturing	$	90,000,000	71%
	Cost of Manufacturing per lb Nylon 66	$	1.59	106%

Table 46 summarizes the differences between the full production and turndown case. The FCI and COL are not changed for the turndown case as the same pieces of equipment are used in production. However, CRM and CUT are directly tied to production rate and so are significantly lower than the full production case. Since the COMd is greater than 67% of the COMd of the full production case, the cost of manufacturing per lb of nylon 66 is greater for the turndown case. This can be attributed to portions of the COMd that scale with FCI and COL, like plant overhead, as these terms would remain the same even as the production rate is decreased. The full production case benefits from an economy of scale.

Economic Analysis:

Table 47: Economic Parameters

Key Parameter	Value
Internal ROR (Hurdle Rate)	15%
Project Evaluation Lifetime	10 Years
Effective Tax Rate (Expense)	40%
Service Factor	0.95

Several key economic parameters have been summarized in Table 47. A hurdle rate of 15% was used as a conservative estimate of the ROR expected in many large companies. A hurdle rate of 7-8% was also considered but the risk involved in investing in polymer production necessitates a larger return than those historically available on the US stock market. Polymer production shares many characteristics with hydrocarbon refining and so a project evaluation lifetime of 10 years was selected. Similarly, the depreciation was calculated using MACRS as if the process was a hydrocarbon refining process. The half year convention was used and the recovery period used was 10 years [14]. An approximate tax rate of 40% was used and a sensitivity analysis was performed on the typical range of US income taxes. The company was assumed to be large enough that an expense tax situation applies. A service factor of 0.95 was selected to allow for frequent cleaning to prevent crystallized nylon buildup and excessive fouling.

Capital costs are incurred during 2017 and 2018 is the first year of planned full production. Working capital costs is incurred during 2018 as part of plant startup. Working capital is approximated to be 5% of the fixed capital investment. This is the lower bound of a 5-10% heuristic due to the lack of expensive catalysts and large holding tanks which are major contributors to high working capital costs. The majority of the working capital is tied up in the polymer melt in the polymerization reactors and the hot oil used to heat these reactors. There is no reason this process cannot continue after the 10 year evaluation lifetime and so no salvage was included in this economic analysis.

The washout assumption was made due to the limited available information regarding current and projected adipic acid, HMDA, and nylon 6,6 prices. The process is very sensitive to changes in the price of both products and reactants as seen in the previous sensitivity analysis. This sensitivity will likely necessitate passing increased costs onto consumers to maintain the projected profit margin. This supports the washout assumption [28].

Payback Period, NPV, and DCFROR Analysis:

The undiscounted and discounted payback periods for the full production and turndown of nylon 6,6 fiber process are summarized in Table 48. The undiscounted payback period is the time it would take for the project to become profitable with a hurdle rate of 0%. The discounted payback period is the time it takes for the project NPV to become positive. The payback periods in Table 48 are very low which indicates that the project is relatively low risk as after approximately 6 months, a positive NPV will still be realized even in the event of the plant shutting down. Since the granular nylon costs more to produce than it is sold for, the undiscounted and discounted payback periods were not able to be calculated. A granular process would never realize a positive NPV, regardless of the hurdle rate.

Table 48: Payback Periods

Nylon 66 Fiber	Undiscounted Payback Period (Months)	Discounted Payback Period (Months)
Full Production	5	6
Turndown	9	10

The calculations for DCFROR and NPV for the granular full production, fiber full production, and fiber turndown cases can be found in Tables 49 - 51. The DCFROR was calculated using the after tax cash flow and the IRR excel function. The NPV was calculated by summing the after tax cash flow after it is discounted by the hurdle rate. The DCFROR of the granular case could not be determined as the granular design never achieves a positive NPV. The large NPV and DCFROR for the nylon fiber production case, $174MM and 243% for the full production case, clearly show that the process is economically desirable. Even during turndown, nylon fiber production is very profitable with an NPV of $98MM and a DCFROR of 145%.

Table 49: Full Granular Production Cash Flow Sheet

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
Nylon 66 Production (lbm/year)		85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000
Nylon 66 Sales Price	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76
Sales Revenue	-	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290
+ Salvage Value											
- Royalties											
Net Revenue	-	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290	64,580,290
-Raw Materials		(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)
-Utilities		(1,291,847)	(1,291,847)	(1,291,847)	(1,291,847)	(1,291,847)	(1,291,847)	(1,291,847)	(1,291,847)	(1,291,847)	(1,291,847)
-Operating Labor		(3,387,760)	(3,387,760)	(3,387,760)	(3,387,760)	(3,387,760)	(3,387,760)	(3,387,760)	(3,387,760)	(3,387,760)	(3,387,760)
-Waste Treatment		(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)
- Other Op Costs		(29,210,557)	(29,210,557)	(29,210,557)	(29,210,557)	(29,210,557)	(29,210,557)	(29,210,557)	(29,210,557)	(29,210,557)	(29,210,557)
- Depreciation		(865,344)	(1,557,620)	(1,246,096)	(996,876)	(797,847)	(637,759)	(566,800)	(566,800)	(567,666)	(566,800)
- Amortization											
- Depletion											
- Loss Forward											
- Writeoff											(716,505)
Taxable Income	-	(61,711,508)	(62,403,784)	(62,092,260)	(61,843,041)	(61,644,012)	(61,483,923)	(61,412,965)	(61,412,965)	(61,413,830)	(62,129,470)
- Tax @40%	-	24,684,603	24,961,514	24,836,904	24,737,216	24,657,605	24,593,569	24,565,186	24,565,186	24,565,532	24,851,788
Net Income	-	(37,026,905)	(37,442,270)	(37,255,356)	(37,105,824)	(36,986,407)	(36,890,354)	(36,847,779)	(36,847,779)	(36,848,298)	(37,277,682)
+ Depreciation	-	865,344	1,557,620	1,246,096	996,876	797,847	637,759	566,800	566,800	567,666	566,800
+ Amortization	-	-	-	-	-	-	-	-	-	-	-
+ Depletion	-	-	-	-	-	-	-	-	-	-	-
+ Loss Forward	-	-	-	-	-	-	-	-	-	-	-
+ Writeoff	-	-	-	-	-	-	-	-	-	-	716,505
- Working Capital		(432,672)									
- Fixed Capital	(8,653,442)										
Cash Flow	(8,653,442)	(36,594,233)	(35,884,651)	(36,009,260)	(36,108,948)	(36,188,560)	(36,252,595)	(36,280,978)	(36,280,978)	(36,280,632)	(35,994,376)
Discount factor (P/Fi,n)	1.000	0.870	0.756	0.658	0.572	0.497	0.432	0.376	0.327	0.284	0.247
Discounted Cash Flow	(8,653,442)	(31,821,072)	(27,133,951)	(23,676,673)	(20,645,408)	(17,992,110)	(15,672,997)	(13,639,364)	(11,860,316)	(10,313,220)	(8,897,259)
NPV @ i* =	(190,305,813)										

Table 50: Full Fiber Production Cash Flow Sheet

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
Nylon 66 Production (lbm/year)		85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000
Nylon 66 Sales Price	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24
Sales Revenue	-	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062
+ Salvage Value											
- Royalties											
Net Revenue	-	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062
-Raw Materials		(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)
-Utilities		(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)
-Operating Labor		(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)
-Waste Treatment		(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)
- Other Op Costs		(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)
- Depreciation		(1,534,973)	(2,762,951)	(2,210,361)	(1,768,289)	(1,415,245)	(1,131,275)	(1,005,407)	(1,005,407)	(1,006,942)	(1,005,407)
- Amortization											
- Depletion											
- Loss Forward											
- Writeoff											(1,270,958)
Taxable Income	-	60,373,058	59,145,080	59,697,670	60,139,742	60,492,786	60,776,756	60,902,623	60,902,623	60,901,088	59,631,666
- Tax @40%	-	(24,149,223)	(23,658,032)	(23,879,068)	(24,055,897)	(24,197,114)	(24,310,702)	(24,361,049)	(24,361,049)	(24,360,435)	(23,852,666)
Net Income	-	36,223,835	35,487,048	35,818,602	36,083,845	36,295,671	36,466,053	36,541,574	36,541,574	36,540,653	35,779,000
+ Depreciation	-	1,534,973	2,762,951	2,210,361	1,768,289	1,415,245	1,131,275	1,005,407	1,005,407	1,006,942	1,005,407
+ Amortization	-	-	-	-	-	-	-	-	-	-	-
+ Depletion	-	-	-	-	-	-	-	-	-	-	-
+ Loss Forward	-	-	-	-	-	-	-	-	-	-	-
+ Writeoff	-	-	-	-	-	-	-	-	-	-	1,270,958
- Working Capital		(767,486)									
- Fixed Capital	(15,349,728)										
Cash Flow	(15,349,728)	36,991,321	38,249,999	38,028,963	37,852,134	37,710,916	37,597,328	37,546,981	37,546,981	37,547,595	38,055,364
Discount factor (P/Fi,n)	1.000	0.870	0.756	0.658	0.572	0.497	0.432	0.376	0.327	0.284	0.247
Discounted Cash Flow	(15,349,728)	32,166,366	28,922,494	25,004,660	21,642,080	18,748,990	16,254,363	14,115,301	12,274,175	10,673,370	9,406,704
NPV @ i* =	173,858,776										
DCFROR =	243%										

Table 51: Turndown Fiber Production Cash Flow Sheet

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
Nylon 66 Production (lbm/year)		56,813,428	56,813,428	56,813,428	56,813,428	56,813,428	56,813,428	56,813,428	56,813,428	56,813,428	56,813,428
Nylon 66 Sales Price	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24
Sales Revenue	-	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742
+ Salvage Value											
- Royalties											
Net Revenue	-	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742	127,115,742
-Raw Materials		(61,328,333)	(61,328,333)	(61,328,333)	(61,328,333)	(61,328,333)	(61,328,333)	(61,328,333)	(61,328,333)	(61,328,333)	(61,328,333)
-Utilities		(1,504,027)	(1,504,027)	(1,504,027)	(1,504,027)	(1,504,027)	(1,504,027)	(1,504,027)	(1,504,027)	(1,504,027)	(1,504,027)
-Operating Labor		(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)
-Waste Treatment		(774)	(774)	(774)	(774)	(774)	(774)	(774)	(774)	(774)	(774)
- Other Op Costs		(23,936,045)	(23,936,045)	(23,936,045)	(23,936,045)	(23,936,045)	(23,936,045)	(23,936,045)	(23,936,045)	(23,936,045)	(23,936,045)
- Depreciation		(1,534,973)	(2,762,951)	(2,210,361)	(1,768,289)	(1,415,245)	(1,131,275)	(1,005,407)	(1,005,407)	(1,006,942)	(1,005,407)
- Amortization											
- Depletion											
- Loss Forward											
- Writeoff											(1,270,958)
Taxable Income	-	35,104,229	33,876,251	34,428,841	34,870,913	35,223,957	35,507,927	35,633,795	35,633,795	35,632,260	34,362,837
- Tax @40%	-	(14,041,692)	(13,550,500)	(13,771,536)	(13,948,365)	(14,089,583)	(14,203,171)	(14,253,518)	(14,253,518)	(14,252,904)	(13,745,135)
Net Income	-	21,062,538	20,325,751	20,657,305	20,922,548	21,134,374	21,304,756	21,380,277	21,380,277	21,379,356	20,617,702
+ Depreciation	-	1,534,973	2,762,951	2,210,361	1,768,289	1,415,245	1,131,275	1,005,407	1,005,407	1,006,942	1,005,407
+ Amortization	-	-	-	-	-	-	-	-	-	-	-
+ Depletion	-	-	-	-	-	-	-	-	-	-	-
+ Loss Forward	-	-	-	-	-	-	-	-	-	-	-
+ Writeoff	-	-	-	-	-	-	-	-	-	-	1,270,958
- Working Capital		(767,486)									
- Fixed Capital	(15,349,728)										
Cash Flow	(15,349,728)	21,830,024	23,088,702	22,867,666	22,690,837	22,549,619	22,436,031	22,385,684	22,385,684	22,386,298	22,894,067
Discount factor (P/Fi,n)	1.000	0.870	0.756	0.658	0.572	0.497	0.432	0.376	0.327	0.284	0.247
Discounted Cash Flow	(15,349,728)	18,982,630	17,458,376	15,035,861	12,973,560	11,211,146	9,699,715	8,415,608	7,317,920	6,363,583	5,659,063
NPV @ i* =	97,767,733										
DCFROR =	145%										

Sensitivity Analysis:

Figure 4 is a tornado chart that summarizes the results of several single variable analyses. Table 52 summarizes the range of values used for each single variable analysis. The range of values was taken from Table 10.1 of Turton and are probable variations for a 10 year project life [31].

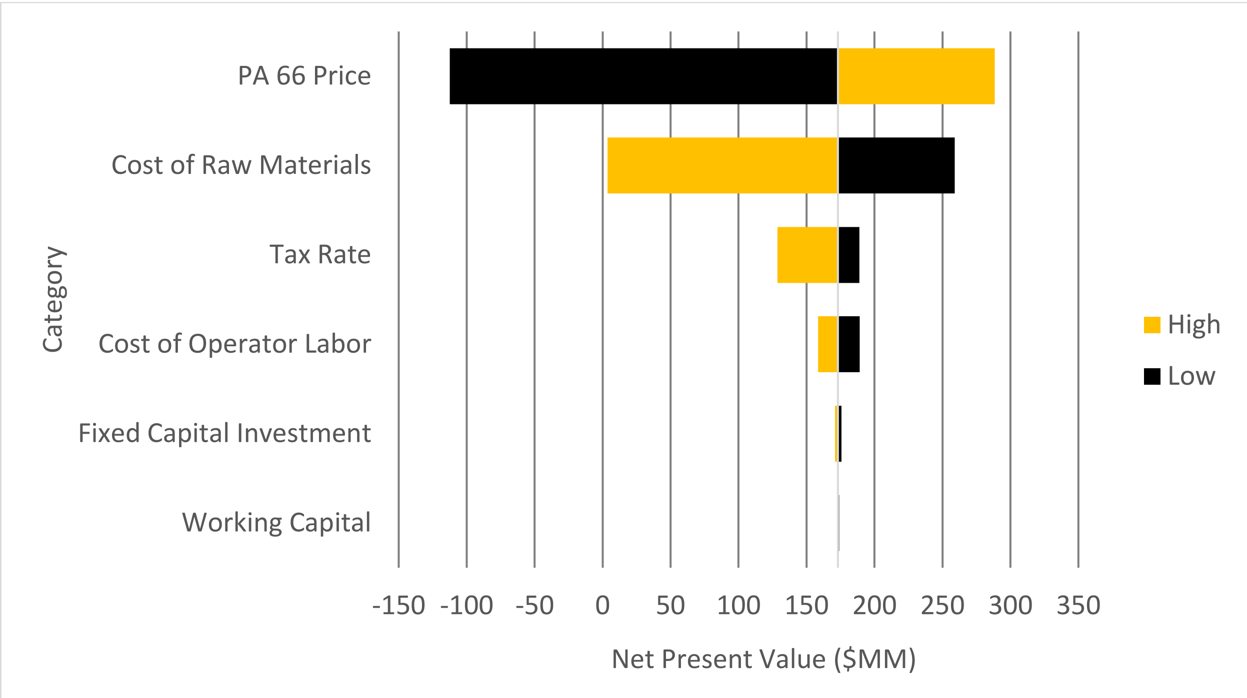

Figure 4: Economic Sensitivity Analysis

Table 52: Sensitivity Analysis Parameters

Variable	Low	High
PA 66 Price	-50%	20%
CRM	-25%	50%
Tax Rate	-5%	15%
COL	-50%	50%
FCI	-20%	30%
Working Capital	-20%	50%

Raw material and nylon 6,6 prices had the most dramatic impact on the NPV of the project. The price of nylon 6,6 is the only single variable analysis that resulted in a negative NPV. This suggests that if the price of nylon 6,6 can be increased as raw material costs rise, the process has little risk of a negative NPV. Securing long term contracts to hedge against future price fluctuations would eliminate the majority of the risk and uncertainty for this design. Research into historical CRM and nylon 6,6 price fluctuations would also serve to increase the understanding of the biggest economic risk to the project.

Variations in the tax rate have a noticeable effect on the project NPV. Consulting with local tax accountants could secure a better tax estimate and reduce the uncertainty of the NPV. Similarly, variations in the COL have a minor but significant effect on the NPV. The effect of the COL uncertainty may be slightly overestimated as the range of COL used in the single variable sensitivity analysis was assumed to be equal to the range of interest rates on Table 10.1 in Turton [31] in the absence of COL information.

Variations in the FCI and the working capital have a negligible effect on the NPV of the process. This means that the relative uncertainty of capital costs based on costing correlations poses little risk to the economic viability of the project as a whole.

Conclusions and Recommendations:

The economic analysis showed that the design to produce nylon 6,6 fibers is economically attractive but the production of granular nylon 6,6 is not economically attractive. Therefore, the design to produce nylon 6,6 fiber should be pursued. This determination was made on the basis of a positive NPV and a DCFROR greater than the hurdle rate of 15%. The turndown production of nylon 6,6 fiber is also economically attractive but features a higher cost of manufacturing per pound of nylon 6,6 produced compared to full scale production.

The sensitivity analysis indicated that the that the production of nylon fibers is sensitive to changes in the sale price of nylon and the raw materials required to produce it. More in depth market research and the establishment of long term contracts can both mitigate the effect of this sensitivity by reducing the uncertainty involved in the chemical prices.

It is also recommended that further research and development is conducted to determine how appropriate the assumptions involving the instantaneous evaporation of water and the non-volatility of HMDA were for a real process. The solubility of the nylon 6,6 salt is another possible area of investigation as the design was limited to the solubility available in literature. Reducing the weight fraction of water to saturate the salt solution could help optimize the process.

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We would like thank Invista for generously providing price quotes for hexamethylene diamine and adipic acid.

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Appendix:

Appendix Table of Contents

List of Tables:

A.1 Reactor Simulation

Reactions:

A + C = L + W (Polymerization Reaction)

C → SE + W (Degradation Reaction 1)

L → SE + A (Degradation Reaction 2)

SE → SB + CO_2 (Degradation Reaction 3)

SB + 2A → X + $2NH_3$ (Degradation Reaction 4)

Where,

A = amine end-group

C = carboxyl end-group

L = amide linkage

SE = stabilized end-group

W = water

SB = Schiff base

X = crosslink

Rate Laws:

For the polymerization reaction, the reaction rate is modeled by Equation A.1. Note that the literature referenced has the total concentration raised to the first power but here the second power is used. This is because the standard form for a second order reversible reaction requires the total concentration term to be squared. This is supported by an analysis of the units, which shows that the term must be squared for the proper units for reaction rate to be produced.

$$R_p = C_t^2 k_p (x_A x_C - \frac{x_l x_w}{K_{ap}}) \qquad \textit{Equation A.25}$$

Where,

R_p = the rate of reaction for the polymerization reaction

C_t = the total concentration in the solution

kp = the rate constant for the forward reaction

x_A = the mole fraction of amine functional groups

x_C = the mole fraction of carboxyl functional groups

x_l = the mole fraction of amide linkages

x_w = the mole fraction of water

K_{ap} = the reverse rate constant

For the first degradation reaction:

$$R_{d1} = C_t k_{d1} x_C \quad \text{Equation A.26}$$

Where

R_{d1} = the rate of reaction for the first degradation reaction

k_{d1} = the rate constant for the first degradation reaction

For the second degradation reaction:

$$R_{d2} = C_t x_l (k_{d2} + k_{d2c} x_A) \quad \text{Equation A.27}$$

Where,

R_{d2} = the rate of reaction for the second degradation reaction

kd_2 = the rate constant for the second degradation reaction

kd_{2c} = the catalyst rate constant for the second degradation reaction

For the third degradation reaction,

$$R_{d3} = C_t k_{d3} x_A x_{SE}^{0.1} \quad \text{Equation A.28}$$

Where,

R_{d3} = the rate of reaction for the third degradation reaction

k_{d3} = the rate constant for the third degradation reaction

x_{SE} = the mole fraction of stable end groups

For the fourth degradation reaction,

$$R_{d4} = C_t k_{d4} x_A x_{SB}^{0.3} \quad \text{Equation A.29}$$

Where,

R_{d4} = the rate of reaction for the fourth degradation reaction

k_{d4} = the rate constant for the first degradation reaction

x_{SB} = the mole fraction of Schiff base

Also used in the simulation were the following equations for other necessary reaction parameters.

$$x_i = \frac{C_i}{C_t}$$ *Equation A.30*

Where,

x_i = the mole fraction of species i

C_i = the concentration of species i

$$C_t = C_A + C_C + C_l + C_W + C_{SE} + C_{SB} + C_X$$ *Equation A.31*

Where,

C_A = the concentration of amine end groups

C_C = the concentration of carboxyl end groups

C_l = the concentration of amine linkages

C_W = the concentration of water

C_{SE} = the concentration of stable end groups

C_{SB} = the concentration of Schiff base

C_X = the concentration of cross linkages

$$k_j = k_{jo}\exp(-\frac{E_j}{R}\left(\frac{1}{T} - \frac{1}{To}\right))$$ *Equation A.32*

Where,

k_j = the rate constant for reaction j

k_{jo} = the reference rate constant for reaction

E_j = the activation energy for reaction j

R = the gas constant

T = the temperature of the reaction

To = the reference temperature of the reaction

$$K_{ap} = K_o\exp(-\frac{\Delta H_{app}}{R}\left(\frac{1}{T} - \frac{1}{T_o}\right))$$ *Equation A.33*

Where,

K_o = the reference K value

ΔH_{app} = the heat of reaction

$$k_{po} = \exp(2.55 - 0.45\tanh(25(x_W - 0.55))) + 8.58(\tanh(50(x_W - 0.10)) - 1)(1 - 30.05x_C) \quad \textit{Equation A.34}$$

Where,

k_{po} = the reference k_p value

$$\Delta H_{app} = 7650\tanh(6.5(x_W - 0.52)) + 6500\exp\left(-\frac{x_W}{0.065}\right) - 800 \quad \textit{Equation A.35}$$

$$K_o = \exp(\left(1 - 0.47\exp\left(-\frac{x_W^{0.5}}{0.2}\right)\right)(8.45 - 4.2x_W)) \quad \textit{Equation A.36}$$

The mole balances for each species was also needed for the model.

$$\frac{d(n_A)}{dt} = Q_{in} * C_{Ao} - R_p + R_{d2} - 2R_{d4} - Q_{out} * C_A \quad \textit{Equation A.37}$$

$$\frac{d(n_C)}{dt} = Q_{in} * C_{Co} - R_p - R_{d1} - Q_{out} * C_C \quad \textit{Equation A.38}$$

$$\frac{d(n_l)}{dt} = Q_{in}C_{lo} + R_p - R_{d2} - Q_{out} * C_l \quad \textit{Equation A.39}$$

$$\frac{d(n_{SB})}{dt} = Q_{in}C_{SB0} + R_{d3} - R_{d4} - Q_{out} * C_{SB} \quad \textit{Equation A.40}$$

$$\frac{d(n_{SE})}{dt} = Q_{in}C_{SEo} + R_{d1} + R_{d2} - R_{d3} - Q_{out} * C_{SE} \quad \textit{Equation A.41}$$

$$\frac{d(n_X)}{dt} = Q_{in}C_{Xo} + R_{d4} - Q_{out} * C_X \quad \textit{Equation A.42}$$

Where,

n_i = the number of moles of species I present

Q_{in} = the volumetric flowrate of the inlet stream

C_{io} = the inlet stream concentration of species i

Q_{out} = the volumetric flowrate of the outlet stream

To find the flowrates of the vent stream and the liquid outlet, mass balances were used as follows.

$$\dot{m}_W = (Q_{in}C_{Wo} + R_p + R_{d1})MW_W \quad \textit{Equation A.43}$$

$$\dot{m}_{CO2} = R_{d3}MW_{CO2} \quad \textit{Equation A.44}$$

$$\dot{m}_{NH3} = 2R_{d4}MW_{NH3} \quad \textit{Equation A.45}$$

$$Q_{out} = \frac{Q_{in}\rho_{in} - (\dot{m}_W + \dot{m}_{CO2} + \dot{m}_{NH3})}{\rho_{out}} \quad \textit{Equation A.46}$$

Where,

$\dot{m}_i$ = the mass flowrate of species i

MW_i = the molecular weight of species i

ρ_{in} = the density of the inlet stream

ρ_{out} = the density of the outlet stream

Polymath Code:

<u>Standard Case – CSTR 1</u>

```
##Notation
	#Rp = rate of reaction for the polymerization reaction
	#Rd1 = rate of reaction for degradation reaction 1
	#Rd2 = rate of reaction for degradation reaction 2
	#Rd3 = rate of reaction for degradation reaction 3
	#Rd4 = rate of reaction for degradation reaction 4
	#T = temperature of the liquid in the tank
	#Qin = volumetric flowrate of the liquid entering the tank
	#rhoin = density of the liquid entering the tank
	#rhoout = density of the liquid leaving the tank
	#tau = residence time of the fluid in the tank
	#V = liquid volume in the tank
	#Ci0 = inlet concentration of species i
	#Ci = bulk liquid concentration of species i
	#ni = number of moles of species i in the tank
	#mdotvent_i = mass flowrate of species i exiting tank as gas through vent
		#i =
			#a for amine end groups
			#c for carboxyl end groups
			#l for amide linkages
			#sb for Sciff base
			#x for cross linkages
			#w for water
			#co2 for carbon dioxide
			#nh3 for ammonia
			#t for total
	#Kap = the equilibrium constant for the polymerization reaction
	#K0 = the reference equilibrium constant for the polymerization reaction
	#kp = the rate constant for the polymerization reaction
	#kp0 = the rate constant reference for the polymerization reaction
	#kd1 = the rate constant for degradation reaction 1
	#kd2 = the rate constant for degradation reaction 2
	#kd2c = the catalyzed rate constant for degradation reaction 2
	#kd3 = the rate constant for degradation reaction 3
	#kd4 = the rate constant for degradation reaction 4
	#deltaH = heat of reaction for the process
	#t = time
```

```
        #Qout = volumetric liquid flowrate of the liquid exiting the tank

##Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap)  #mol/hr
Rd1=Ct*kd1*(Cc/Ct)  #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct))  #mol/hr
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1)  #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3)  #mol/hr

##Parameters
T=601.15  #K
Qin= 8255  #L/hr
rhoin= 0.97 #kg/L
rhoout=0.88  #kg/L
tau= 3  #hr
V=tau*Qin  #L

##Inlet Concentrations
Ca0= 5  #mol/L
Cc0= 5  #mol/L
Cl0= 0  #mol/L
Csb0= 0  #mol/L
Cse0= 0  #mol/L
Cx0=0  #mol/L
Cw0=17.8  #mol/L

##Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

##Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct)) #L/hr

##Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
```

na(0) = 122825 #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc #mol/hr
nc(0) = 122825 #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl #mol/hr
nl(0) = 0 #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb #mol/hr
nsb(0) = 0.0001 #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse #mol/hr
nse(0) = 0 #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx #mol/hr
nx(0) = 0 #mol
d(nnh3) / d(t) = 0 #mol/hr
nnh3(0) = 0 #mol
d(nco2) / d(t) = 0 #mol/hr
nco2(0) = 0 #mol
d(nw) / d(t) = 0 #mol/hr
nw(0) = 0 #mol

##Outlet Flowrates
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000 #kg/hr
mdotvent_co2=Rd3*44.01/1000 #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000 #kg/hr

##Simulation Times
t(0)=0 #hr
t(f)=50 #hr

<u>Standard Case – CSTR 2</u>

##Notation
    #Rp = rate of reaction for the polymerization reaction
    #Rd1 = rate of reaction for degradation reaction 1
    #Rd2 = rate of reaction for degradation reaction 2
    #Rd3 = rate of reaction for degradation reaction 3
    #Rd4 = rate of reaction for degradation reaction 4
    #T = temperature of the liquid in the tank
    #Qin = volumetric flowrate of the liquid entering the tank
    #rhoin = density of the liquid entering the tank
    #rhoout = density of the liquid leaving the tank
    #tau = residence time of the fluid in the tank
    #V = liquid volume in the tank
    #Ci0 = inlet concentration of species i
    #Ci = bulk liquid concentration of species i
    #ni = number of moles of species i in the tank
    #mdotvent_i = mass flowrate of species i exiting tank as gas through vent
        #i =
            #a for amine end groups
            #c for carboxyl end groups

```
                #l for amide linkages
                #sb for Sciff base
                #x for cross linkages
                #w for water
                #co2 for carbon dioxide
                #nh3 for ammonia
                #t for total
        #Kap = the equilibrium constant for the polymerization reaction
        #K0 = the reference equilibrium constant for the polymerization reaction
        #kp = the rate constant for the polymerization reaction
        #kp0 = the rate constant reference for the polymerization reaction
        #kd1 = the rate constant for degradation reaction 1
        #kd2 = the rate constant for degradation reaction 2
        #kd2c = the catalyzed rate constant for degradation reaction 2
        #kd3 = the rate constant for degradation reaction 3
        #kd4 = the rate constant for degradation reaction 4
        #deltaH = heat of reaction for the process
        #t = time
        #Qout = volumetric liquid flowrate of the liquid exiting the tank

#Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap)  #mol/hr
Rd1=Ct*kd1*(Cc/Ct)  #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct))  #mol/hr
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1)  #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3)  #mol/hr

#Parameters
T=601.15  #K
Qin= 5427  #L/hr
rhoin= 0.88 #kg/L
rhoout=0.92  #kg/L
tau= 3  #hr
V=tau*Qin  #L

#Inlet Concentrations
Ca0= 1.637  #mol/L
Cc0= 1.637  #mol/L
Cl0= 5.968  #mol/L
Csb0= 0  #mol/L
Cse0= 0.0002206  #mol/L
Cx0=0.000051  #mol/L
Cw0=0  #mol/L

#Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
```

```
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

#Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct)) #L/hr

#Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
na(0) = 26654  #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc  #mol/hr
nc(0) = 26651  #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl  #mol/hr
nl(0) = 97169  #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb  #mol/hr
nsb(0) =  0.000001  #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse  #mol/hr
nse(0) =  3.59  #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx  #mol/hr
nx(0) = 0.83  #mol
d(nnh3) / d(t) = 0  #mol/hr
nnh3(0) = 0  #mol
d(nco2) / d(t) = 0  #mol/hr
nco2(0) = 0  #mol
d(nw) / d(t) = 0  #mol/hr
nw(0) = 0  #mol

#Outlet Flowrates
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout  #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000  #kg/hr
mdotvent_co2=Rd3*44.01/1000  #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000  #kg/hr

#Simulation Times
t(0)=0  #hr
t(f)=50  #hr
```

<u>Standard Case – CSTR 3</u>

```
##Notation
```

```
        #Rp = rate of reaction for the polymerization reaction
        #Rd1 = rate of reaction for degradation reaction 1
        #Rd2 = rate of reaction for degradation reaction 2
        #Rd3 = rate of reaction for degradation reaction 3
        #Rd4 = rate of reaction for degradation reaction 4
        #T = temperature of the liquid in the tank
        #Qin = volumetric flowrate of the liquid entering the tank
        #rhoin = density of the liquid entering the tank
        #rhoout = density of the liquid leaving the tank
        #tau = residence time of the fluid in the tank
        #V = liquid volume in the tank
        #Ci0 = inlet concentration of species i
        #Ci = bulk liquid concentration of species i
        #ni = number of moles of species i in the tank
        #mdotvent_i = mass flowrate of species i exiting tank as gas through vent
                #i =
                        #a for amine end groups
                        #c for carboxyl end groups
                        #l for amide linkages
                        #sb for Sciff base
                        #x for cross linkages
                        #w for water
                        #co2 for carbon dioxide
                        #nh3 for ammonia
                        #t for total
        #Kap = the equilibrium constant for the polymerization reaction
        #K0 = the reference equilibrium constant for the polymerization reaction
        #kp = the rate constant for the polymerization reaction
        #kp0 = the rate constant reference for the polymerization reaction
        #kd1 = the rate constant for degradation reaction 1
        #kd2 = the rate constant for degradation reaction 2
        #kd2c = the catalyzed rate constant for degradation reaction 2
        #kd3 = the rate constant for degradation reaction 3
        #kd4 = the rate constant for degradation reaction 4
        #deltaH = heat of reaction for the process
        #t = time
        #Qout = volumetric liquid flowrate of the liquid exiting the tank

#Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap)  #mol/hr
Rd1=Ct*kd1*(Cc/Ct)  #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct))  #mol/hr
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1)  #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3)  #mol/hr

#Parameters
T=601.15  #K
Qin= 5101  #L/hr
rhoin= 0.92 #kg/L
rhoout=0.93  #kg/L
tau= 3  #hr
```

```
V=tau*Qin  #L

#Inlet Concentrations
Ca0= 0.838  #mol/L
Cc0= 0.837  #mol/L
Cl0= 7.254  #mol/L
Csb0= 0  #mol/L
Cse0= 0.0003883  #mol/L
Cx0=0.000084  #mol/L
Cw0=0  #mol/L

#Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

#Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct)) #L/hr

#Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
na(0) = 12816  #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc  #mol/hr
nc(0) = 12814  #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl  #mol/hr
nl(0) = 111000  #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb  #mol/hr
nsb(0) =  0.000001  #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse  #mol/hr
nse(0) =  5.94  #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx  #mol/hr
nx(0) = 1.28  #mol
d(nnh3) / d(t) = 0  #mol/hr
nnh3(0) = 0  #mol
d(nco2) / d(t) = 0  #mol/hr
nco2(0) = 0  #mol
```

```
d(nw) / d(t) = 0  #mol/hr
nw(0) = 0  #mol

#Outlet Flowrates
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout  #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000  #kg/hr
mdotvent_co2=Rd3*44.01/1000  #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000  #kg/hr

#Simulation Times
t(0)=0  #hr
t(f)=50  #hr
```

<u>Standard Case – CSTR 4</u>

```
##Notation
	#Rp = rate of reaction for the polymerization reaction
	#Rd1 = rate of reaction for degradation reaction 1
	#Rd2 = rate of reaction for degradation reaction 2
	#Rd3 = rate of reaction for degradation reaction 3
	#Rd4 = rate of reaction for degradation reaction 4
	#T = temperature of the liquid in the tank
	#Qin = volumetric flowrate of the liquid entering the tank
	#rhoin = density of the liquid entering the tank
	#rhoout = density of the liquid leaving the tank
	#tau = residence time of the fluid in the tank
	#V = liquid volume in the tank
	#Ci0 = inlet concentration of species i
	#Ci = bulk liquid concentration of species i
	#ni = number of moles of species i in the tank
	#mdotvent_i = mass flowrate of species i exiting tank as gas through vent
		#i =
			#a for amine end groups
			#c for carboxyl end groups
			#l for amide linkages
			#sb for Sciff base
			#x for cross linkages
			#w for water
			#co2 for carbon dioxide
			#nh3 for ammonia
			#t for total
	#Kap = the equilibrium constant for the polymerization reaction
	#K0 = the reference equilibrium constant for the polymerization reaction
	#kp = the rate constant for the polymerization reaction
	#kp0 = the rate constant reference for the polymerization reaction
	#kd1 = the rate constant for degradation reaction 1
	#kd2 = the rate constant for degradation reaction 2
	#kd2c = the catalyzed rate constant for degradation reaction 2
```

```
    #kd3 = the rate constant for degradation reaction 3
    #kd4 = the rate constant for degradation reaction 4
    #deltaH = heat of reaction for the process
    #t = time
    #Qout = volumetric liquid flowrate of the liquid exiting the tank

#Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap)  #mol/hr
Rd1=Ct*kd1*(Cc/Ct)  #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct))  #mol/hr
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1)  #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3)  #mol/hr

#Parameters
T=601.15  #K
Qin= 5018  #L/hr
rhoin= 0.93 #kg/L
rhoout=0.94  #kg/L
tau= 3  #hr
V=tau*Qin  #L

#Inlet Concentrations
Ca0= 0.562  #mol/L
Cc0= 0.561  #mol/L
Cl0= 7.663  #mol/L
Csb0= 0  #mol/L
Cse0= 0.0005124  #mol/L
Cx0=0.000106  #mol/L
Cw0=0  #mol/L

#Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

#Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
```

```
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct)) #L/hr

#Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
na(0) = 8468  #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc  #mol/hr
nc(0) = 8451  #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl  #mol/hr
nl(0) = 115363  #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb  #mol/hr
nsb(0) =  0.000001  #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse  #mol/hr
nse(0) =  7.71  #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx  #mol/hr
nx(0) = 1.6  #mol
d(nnh3) / d(t) = 0  #mol/hr
nnh3(0) = 0  #mol
d(nco2) / d(t) = 0  #mol/hr
nco2(0) = 0  #mol
d(nw) / d(t) = 0  #mol/hr
nw(0) = 0  #mol

#Outlet Flows
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout  #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000  #kg/hr
mdotvent_co2=Rd3*44.01/1000  #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000  #kg/hr

#Simulation Times
t(0)=0  #hr
t(f)=50  #hr
```

<u>Standard Case – CSTR 5</u>

```
##Notation
	#Rp = rate of reaction for the polymerization reaction
	#Rd1 = rate of reaction for degradation reaction 1
	#Rd2 = rate of reaction for degradation reaction 2
	#Rd3 = rate of reaction for degradation reaction 3
	#Rd4 = rate of reaction for degradation reaction 4
	#T = temperature of the liquid in the tank
	#Qin = volumetric flowrate of the liquid entering the tank
	#rhoin = density of the liquid entering the tank
	#rhoout = density of the liquid leaving the tank
	#tau = residence time of the fluid in the tank
	#V = liquid volume in the tank
	#Ci0 = inlet concentration of species i
	#Ci = bulk liquid concentration of species i
	#ni = number of moles of species i in the tank
```

```
        #mdotvent_i = mass flowrate of species i exiting tank as gas through vent
                #i =
                        #a for amine end groups
                        #c for carboxyl end groups
                        #l for amide linkages
                        #sb for Sciff base
                        #x for cross linkages
                        #w for water
                        #co2 for carbon dioxide
                        #nh3 for ammonia
                        #t for total
        #Kap = the equilibrium constant for the polymerization reaction
        #K0 = the reference equilibrium constant for the polymerization reaction
        #kp = the rate constant for the polymerization reaction
        #kp0 = the rate constant reference for the polymerization reaction
        #kd1 = the rate constant for degradation reaction 1
        #kd2 = the rate constant for degradation reaction 2
        #kd2c = the catalyzed rate constant for degradation reaction 2
        #kd3 = the rate constant for degradation reaction 3
        #kd4 = the rate constant for degradation reaction 4
        #deltaH = heat of reaction for the process
        #t = time
        #Qout = volumetric liquid flowrate of the liquid exiting the tank

#Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap)  #mol/hr
Rd1=Ct*kd1*(Cc/Ct)  #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct))  #mol/hr
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1)  #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3)  #mol/hr

#Parameters
T=601.15  #K
Qin= 4952  #L/hr
rhoin= 0.94 #kg/L
rhoout=0.94  #kg/L
tau= 3  #hr
V=tau*Qin  #L

#Inlet Concentrations
Ca0= 0.433  #mol/L
Cc0= 0.432  #mol/L
Cl0= 7.903  #mol/L
Csb0= 0  #mol/L
Cse0= 0.0006184  #mol/L
Cx0=0.000124  #mol/L
Cw0=0  #mol/L

#Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
```

```
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

#Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct)) #L/hr

#Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
na(0) = 6427  #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc  #mol/hr
nc(0) = 6411  #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl  #mol/hr
nl(0) = 117391  #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb  #mol/hr
nsb(0) =  0.000001  #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse  #mol/hr
nse(0) =  9.19  #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx  #mol/hr
nx(0) = 1.84  #mol
d(nnh3) / d(t) = 0  #mol/hr
nnh3(0) = 0  #mol
d(nco2) / d(t) = 0  #mol/hr
nco2(0) = 0  #mol
d(nw) / d(t) = 0  #mol/hr
nw(0) = 0  #mol

#Outlet Flowrates
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout  #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000  #kg/hr
mdotvent_co2=Rd3*44.01/1000  #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000  #kg/hr

#Simulation Times
t(0)=0  #hr
t(f)=50  #hr
```

Reduced Case – CSTR 1

##Notation

    #Rp = rate of reaction for the polymerization reaction
    #Rd1 = rate of reaction for degradation reaction 1
    #Rd2 = rate of reaction for degradation reaction 2
    #Rd3 = rate of reaction for degradation reaction 3
    #Rd4 = rate of reaction for degradation reaction 4
    #T = temperature of the liquid in the tank
    #Qin = volumetric flowrate of the liquid entering the tank
    #rhoin = density of the liquid entering the tank
    #rhoout = density of the liquid leaving the tank
    #tau = residence time of the fluid in the tank
    #V = liquid volume in the tank
    #Ci0 = inlet concentration of species i
    #Ci = bulk liquid concentration of species i
    #ni = number of moles of species i in the tank
    #mdotvent_i = mass flowrate of species i exiting tank as gas through vent
        #i =
            #a for amine end groups
            #c for carboxyl end groups
            #l for amide linkages
            #sb for Sciff base
            #x for cross linkages
            #w for water
            #co2 for carbon dioxide
            #nh3 for ammonia
            #t for total
    #Kap = the equilibrium constant for the polymerization reaction
    #K0 = the reference equilibrium constant for the polymerization reaction
    #kp = the rate constant for the polymerization reaction
    #kp0 = the rate constant reference for the polymerization reaction
    #kd1 = the rate constant for degradation reaction 1
    #kd2 = the rate constant for degradation reaction 2
    #kd2c = the catalyzed rate constant for degradation reaction 2
    #kd3 = the rate constant for degradation reaction 3
    #kd4 = the rate constant for degradation reaction 4
    #deltaH = heat of reaction for the process
    #t = time
    #Qout = volumetric liquid flowrate of the liquid exiting the tank

##Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap) #mol/hr
Rd1=Ct*kd1*(Cc/Ct) #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct)) #mol/hr
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1) #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3) #mol/hr

##Parameters

```
T=601.15  #K
Qin= 5531  #L/hr
rhoin= 0.97 #kg/L
rhoout=0.89  #kg/L
tau= 3  #hr
V=tau*Qin  #L

##Inlet Concentrations
Ca0= 5  #mol/L
Cc0= 5  #mol/L
Cl0= 0  #mol/L
Csb0= 0  #mol/L
Cse0= 0  #mol/L
Cx0=0  #mol/L
Cw0=17.8  #mol/L

##Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

##Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct)) #L/hr

##Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
na(0) = 82293  #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc  #mol/hr
nc(0) = 82293  #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl  #mol/hr
nl(0) = 0  #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb  #mol/hr
nsb(0) =  0.0001  #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse  #mol/hr
nse(0) =  0  #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx  #mol/hr
```

```
nx(0) = 0  #mol
d(nnh3) / d(t) = 0  #mol/hr
nnh3(0) = 0  #mol
d(nco2) / d(t) = 0  #mol/hr
nco2(0) = 0  #mol
d(nw) / d(t) = 0  #mol/hr
nw(0) = 0  #mol

##Outlet Flowrates
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout  #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000  #kg/hr
mdotvent_co2=Rd3*44.01/1000  #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000  #kg/hr

##Simulation Times
t(0)=0  #hr
t(f)=50  #hr
```

<u>Reduced Case – CSTR 2</u>

```
##Notation
	#Rp = rate of reaction for the polymerization reaction
	#Rd1 = rate of reaction for degradation reaction 1
	#Rd2 = rate of reaction for degradation reaction 2
	#Rd3 = rate of reaction for degradation reaction 3
	#Rd4 = rate of reaction for degradation reaction 4
	#T = temperature of the liquid in the tank
	#Qin = volumetric flowrate of the liquid entering the tank
	#rhoin = density of the liquid entering the tank
	#rhoout = density of the liquid leaving the tank
	#tau = residence time of the fluid in the tank
	#V = liquid volume in the tank
	#Ci0 = inlet concentration of species i
	#Ci = bulk liquid concentration of species i
	#ni = number of moles of species i in the tank
	#mdotvent_i = mass flowrate of species i exiting tank as gas through vent
		#i =
			#a for amine end groups
			#c for carboxyl end groups
			#l for amide linkages
			#sb for Sciff base
			#x for cross linkages
			#w for water
			#co2 for carbon dioxide
			#nh3 for ammonia
			#t for total
	#Kap = the equilibrium constant for the polymerization reaction
	#K0 = the reference equilibrium constant for the polymerization reaction
```

```
    #kp = the rate constant for the polymerization reaction
    #kp0 = the rate constant reference for the polymerization reaction
    #kd1 = the rate constant for degradation reaction 1
    #kd2 = the rate constant for degradation reaction 2
    #kd2c = the catalyzed rate constant for degradation reaction 2
    #kd3 = the rate constant for degradation reaction 3
    #kd4 = the rate constant for degradation reaction 4
    #deltaH = heat of reaction for the process
    #t = time
    #Qout = volumetric liquid flowrate of the liquid exiting the tank

##Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap)  #mol/hr
Rd1=Ct*kd1*(Cc/Ct)  #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct))  #mol/hr
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1)  #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3)  #mol/hr

##Parameters
T=601.15  #K
Qin= 3579  #L/hr
rhoin= 0.89 #kg/L
rhoout=0.93  #kg/L
tau= 3  #hr
V=tau*Qin  #L

##Inlet Concentrations
Ca0= 1.444  #mol/L
Cc0= 1.444  #mol/L
Cl0= 6.282  #mol/L
Csb0= 0  #mol/L
Cse0= 0.0003104  #mol/L
Cx0=0.00007  #mol/L
Cw0=0  #mol/L

##Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

##Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
```

```
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct)) #L/hr

##Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
na(0) = 15506  #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc  #mol/hr
nc(0) = 15504  #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl  #mol/hr
nl(0) = 67457  #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb  #mol/hr
nsb(0) =  0.0001  #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse  #mol/hr
nse(0) =  3.33  #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx  #mol/hr
nx(0) = 0.76  #mol
d(nnh3) / d(t) = 0  #mol/hr
nnh3(0) = 0  #mol
d(nco2) / d(t) = 0  #mol/hr
nco2(0) = 0  #mol
d(nw) / d(t) = 0  #mol/hr
nw(0) = 0  #mol

##Outlet Flowrates
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout  #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000  #kg/hr
mdotvent_co2=Rd3*44.01/1000  #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000  #kg/hr

##Simulation Times
t(0)=0  #hr
t(f)=50  #hr
```

<u>Reduced Capacity – CSTR 3</u>

```
##Notation
	#Rp = rate of reaction for the polymerization reaction
	#Rd1 = rate of reaction for degradation reaction 1
	#Rd2 = rate of reaction for degradation reaction 2
	#Rd3 = rate of reaction for degradation reaction 3
	#Rd4 = rate of reaction for degradation reaction 4
	#T = temperature of the liquid in the tank
	#Qin = volumetric flowrate of the liquid entering the tank
	#rhoin = density of the liquid entering the tank
	#rhoout = density of the liquid leaving the tank
```

```
	#tau = residence time of the fluid in the tank
	#V = liquid volume in the tank
	#Ci0 = inlet concentration of species i
	#Ci = bulk liquid concentration of species i
	#ni = number of moles of species i in the tank
	#mdotvent_i = mass flowrate of species i exiting tank as gas through vent
		#i =
			#a for amine end groups
			#c for carboxyl end groups
			#l for amide linkages
			#sb for Sciff base
			#x for cross linkages
			#w for water
			#co2 for carbon dioxide
			#nh3 for ammonia
			#t for total
	#Kap = the equilibrium constant for the polymerization reaction
	#K0 = the reference equilibrium constant for the polymerization reaction
	#kp = the rate constant for the polymerization reaction
	#kp0 = the rate constant reference for the polymerization reaction
	#kd1 = the rate constant for degradation reaction 1
	#kd2 = the rate constant for degradation reaction 2
	#kd2c = the catalyzed rate constant for degradation reaction 2
	#kd3 = the rate constant for degradation reaction 3
	#kd4 = the rate constant for degradation reaction 4
	#deltaH = heat of reaction for the process
	#t = time
	#Qout = volumetric liquid flowrate of the liquid exiting the tank

##Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap)  #mol/hr
Rd1=Ct*kd1*(Cc/Ct)  #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct))  #mol/hr
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1)  #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3)  #mol/hr

##Parameters
T=601.15  #K
Qin= 3371  #L/hr
rhoin= 0.93 #kg/L
rhoout=0.94  #kg/L
tau= 3  #hr
V=tau*Qin  #L

##Inlet Concentrations
Ca0= 0.712  #mol/L
Cc0= 0.712  #mol/L
Cl0= 7.668  #mol/L
Csb0= 0  #mol/L
Cse0= 0.000535  #mol/L
Cx0=0.000113  #mol/L
```

```
Cw0=0  #mol/L

##Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

##Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct)) #L/hr

##Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
na(0) = 7204  #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc  #mol/hr
nc(0) = 7202  #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl  #mol/hr
nl(0) = 77546  #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb  #mol/hr
nsb(0) =  0.0001  #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse  #mol/hr
nse(0) =  5.41  #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx  #mol/hr
nx(0) = 1.14  #mol
d(nnh3) / d(t) = 0  #mol/hr
nnh3(0) = 0  #mol
d(nco2) / d(t) = 0  #mol/hr
nco2(0) = 0  #mol
d(nw) / d(t) = 0  #mol/hr
nw(0) = 0  #mol

##Outlet Flowrates
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout  #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000  #kg/hr
mdotvent_co2=Rd3*44.01/1000  #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000  #kg/hr
```

##Simulation Times
t(0)=0 #hr
t(f)=50 #hr

<u>Reduced Capacity – CSTR 4</u>

##Notation
#Rp = rate of reaction for the polymerization reaction
#Rd1 = rate of reaction for degradation reaction 1
#Rd2 = rate of reaction for degradation reaction 2
#Rd3 = rate of reaction for degradation reaction 3
#Rd4 = rate of reaction for degradation reaction 4
#T = temperature of the liquid in the tank
#Qin = volumetric flowrate of the liquid entering the tank
#rhoin = density of the liquid entering the tank
#rhoout = density of the liquid leaving the tank
#tau = residence time of the fluid in the tank
#V = liquid volume in the tank
#Ci0 = inlet concentration of species i
#Ci = bulk liquid concentration of species i
#ni = number of moles of species i in the tank
#mdotvent_i = mass flowrate of species i exiting tank as gas through vent
#i =
#a for amine end groups
#c for carboxyl end groups
#l for amide linkages
#sb for Sciff base
#x for cross linkages
#w for water
#co2 for carbon dioxide
#nh3 for ammonia
#t for total
#Kap = the equilibrium constant for the polymerization reaction
#K0 = the reference equilibrium constant for the polymerization reaction
#kp = the rate constant for the polymerization reaction
#kp0 = the rate constant reference for the polymerization reaction
#kd1 = the rate constant for degradation reaction 1
#kd2 = the rate constant for degradation reaction 2
#kd2c = the catalyzed rate constant for degradation reaction 2
#kd3 = the rate constant for degradation reaction 3
#kd4 = the rate constant for degradation reaction 4
#deltaH = heat of reaction for the process
#t = time
#Qout = volumetric liquid flowrate of the liquid exiting the tank

##Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap) #mol/hr
Rd1=Ct*kd1*(Cc/Ct) #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct)) #mol/hr

```
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1)  #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3)  #mol/hr

##Parameters
T=601.15  #K
Qin= 3319  #L/hr
rhoin= 0.94 #kg/L
rhoout=0.94  #kg/L
tau= 3  #hr
V=tau*Qin  #L

##Inlet Concentrations
Ca0= 0.469  #mol/L
Cc0= 0.469  #mol/L
Cl0= 8.042  #mol/L
Csb0= 0  #mol/L
Cse0= 0.0007008  #mol/L
Cx0=0.000142  #mol/L
Cw0=0  #mol/L

##Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

##Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct))  #L/hr

##Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
na(0) = 4672  #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc  #mol/hr
nc(0) = 4671  #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl  #mol/hr
nl(0) = 80074  #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb  #mol/hr
```

```
nsb(0) =  0.0001  #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse  #mol/hr
nse(0) =  6.98  #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx  #mol/hr
nx(0) = 1.41  #mol
d(nnh3) / d(t) = 0  #mol/hr
nnh3(0) = 0  #mol
d(nco2) / d(t) = 0  #mol/hr
nco2(0) = 0  #mol
d(nw) / d(t) = 0  #mol/hr
nw(0) = 0  #mol

##Outlet Flowrates
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout  #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000  #kg/hr
mdotvent_co2=Rd3*44.01/1000  #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000  #kg/hr

##Simulation Times
t(0)=0  #hr
t(f)=50  #hr
```

<u>Reduced Capacity – CSTR 5</u>

```
##Notation
        #Rp = rate of reaction for the polymerization reaction
        #Rd1 = rate of reaction for degradation reaction 1
        #Rd2 = rate of reaction for degradation reaction 2
        #Rd3 = rate of reaction for degradation reaction 3
        #Rd4 = rate of reaction for degradation reaction 4
        #T = temperature of the liquid in the tank
        #Qin = volumetric flowrate of the liquid entering the tank
        #rhoin = density of the liquid entering the tank
        #rhoout = density of the liquid leaving the tank
        #tau = residence time of the fluid in the tank
        #V = liquid volume in the tank
        #Ci0 = inlet concentration of species i
        #Ci = bulk liquid concentration of species i
        #ni = number of moles of species i in the tank
        #mdotvent_i = mass flowrate of species i exiting tank as gas through vent
                #i =
                        #a for amine end groups
                        #c for carboxyl end groups
                        #l for amide linkages
                        #sb for Schiff base
                        #x for cross linkages
                        #w for water
                        #co2 for carbon dioxide
                        #nh3 for ammonia
```

```
                    #t for total
        #Kap = the equilibrium constant for the polymerization reaction
        #K0 = the reference equilibrium constant for the polymerization reaction
        #kp = the rate constant for the polymerization reaction
        #kp0 = the rate constant reference for the polymerization reaction
        #kd1 = the rate constant for degradation reaction 1
        #kd2 = the rate constant for degradation reaction 2
        #kd2c = the catalyzed rate constant for degradation reaction 2
        #kd3 = the rate constant for degradation reaction 3
        #kd4 = the rate constant for degradation reaction 4
        #deltaH = heat of reaction for the process
        #t = time
        #Qout = volumetric liquid flowrate of the liquid exiting the tank

##Reaction Rate Laws
Rp=(Ct^2)*kp*((Ca/Ct)*(Cc/Ct)-(Cl/Ct)*(Cw/Ct)/Kap)  #mol/hr
Rd1=Ct*kd1*(Cc/Ct)  #mol/hr
Rd2=Ct*(Cl/Ct)*(kd2+kd2c*(Ca/Ct))  #mol/hr
Rd3=Ct*kd3*(Ca/Ct)*((Cse/Ct)^0.1)  #mol/hr
Rd4=Ct*kd4*(Ca/Ct)*((Csb/Ct)^0.3)  #mol/hr

##Parameters
T=601.15  #K
Qin= 3312  #L/hr
rhoin= 0.94 #kg/L
rhoout=0.95  #kg/L
tau= 3  #hr
V=tau*Qin  #L

##Inlet Concentrations
Ca0= 0.355  #mol/L
Cc0= 0.355  #mol/L
Cl0= 8.175  #mol/L
Csb0= 0  #mol/L
Cse0= 0.0008323  #mol/L
Cx0=0.000163  #mol/L
Cw0=0  #mol/L

##Bulk Fluid Concentrations
Ca=na/V  #mol/L
Cw=nw/V  #mol/L
Cl=nl/V  #mol/L
Cse=nse/V  #mol/L
Cc= nc/V  #mol/L
Csb=nsb/V  #mol/L
Cx=nx/V  #mol/L
Ct=(Ca+Cc+Cl+Cw+Cse+Cx+Csb)  #mol/L

##Rate Law Terms
Kap=K0*exp(-deltaH*(1/T-1/473)/0.001987)  #unitless
kp=kp0*exp(-21.4*(1/T-1/473)/0.001987)  #L/hr
```

```
kd1=0.06*exp(-30*(1/T-1/566)/0.001987)  #L/hr
kd2=0.005*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd2c=0.32*exp(-30*(1/T-1/578)/0.001987)  #L/hr
kd3=0.35*exp(-10*(1/T-1/578)/0.001987)  #L/hr
kd4=10*exp(-50*(1/T-1/578)/0.001987)  #L/hr
K0=exp((1-0.47*exp(-((Cw/Ct)^0.5)/0.2))*(8.45-4.2*(Cw/Ct)))  #unitless
deltaH=7650*tanh(6.5*((Cw/Ct)-0.52))+6500*exp(-(Cw/Ct)/0.065)-800  #kcal/mol
kp0= exp(2.55-0.45*(tanh(25*((Cw/Ct)-0.55))))+8.58*(tanh(50*((Cw/Ct)-0.1))-1)*(1-
30.05*(Cc/Ct))  #L/hr

##Species Mole Differentials
d(na) / d(t) =  Qin*Ca0+(-Rp+Rd2-2*Rd4)-Qout*Ca  #mol/hr
na(0) = 3529  #mol
d(nc) / d(t) = Qin*Cc0+(-Rp-Rd1)-Qout*Cc  #mol/hr
nc(0) = 3528  #mol
d(nl) / d(t) = Qin*Cl0+(Rp-Rd2)-Qout*Cl  #mol/hr
nl(0) = 81215  #mol
d(nsb) / d(t) = Qin*Csb0+(Rd3-Rd4)-Qout*Csb  #mol/hr
nsb(0) =  0  #mol
d(nse) / d(t) = Qin*Cse0+(Rd1+Rd2-Rd3)-Qout*Cse  #mol/hr
nse(0) =  8.27  #mol
d(nx) / d(t) = Qin*Cx0+Rd4-Qout*Cx  #mol/hr
nx(0) = 1.62  #mol
d(nnh3) / d(t) = 0  #mol/hr
nnh3(0) = 0  #mol
d(nco2) / d(t) = 0  #mol/hr
nco2(0) = 0  #mol
d(nw) / d(t) = 0  #mol/hr
nw(0) = 0  #mol

##Outlet Flowrates
Qout=(Qin*rhoin-(mdotvent_w+mdotvent_nh3+mdotvent_co2))/rhoout  #L/hr
mdotvent_w=(Qin*Cw0+Rp+Rd1)*18.02/1000  #kg/hr
mdotvent_co2=Rd3*44.01/1000  #kg/hr
mdotvent_nh3=2*Rd4*17.03/1000  #kg/hr

##Simulation Times
t(0)=0  #hr
t(f)=50  #hr
```

Polymath Results

Table A.53: Polymath Result Standard Case CSTR 1

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	4.95962	1.54851	4.95962	1.637118
2	Ca0	5.	5.	5.	5.
3	Cc	4.95962	1.548454	4.95962	1.636949

4	Cc0	5.	5.	5.	5.
5	Cl	0	0	5.968171	5.968171
6	Cl0	0	0	0	0
7	Csb	4.038E-09	4.038E-09	4.257E-08	4.257E-08
8	Csb0	0	0	0	0
9	Cse	0	0	0.0002206	0.0002206
10	Cse0	0	0	0	0
11	Ct	9.919241	7.400713	9.919241	9.242509
12	Cw	0	0	0	0
13	Cw0	17.8	17.8	17.8	17.8
14	Cx	0	0	5.089E-05	5.089E-05
15	Cx0	0	0	0	0
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155
22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	3.344E+04	1.209E+04	3.344E+04	1.209E+04
25	kp0	260.7436	94.25079	260.7436	94.25079
26	mdotvent_co2	0	0	0.012165	0.012165
27	mdotvent_nh3	0.0137628	0.0079772	0.0137628	0.0094068
28	mdotvent_w	1.747E+04	3231.291	1.747E+04	3231.53
29	na	1.228E+05	3.835E+04	1.228E+05	4.054E+04
30	nc	1.228E+05	3.835E+04	1.228E+05	4.054E+04
31	nco2	0	0	0	0
32	nl	0	0	1.478E+05	1.478E+05
33	nnh3	0	0	0	0
34	nsb	0.0001	0.0001	0.0010543	0.0010543
35	nse	0	0	5.464119	5.464119
36	nw	0	0	0	0
37	nx	0	0	1.260219	1.260219
38	Qin	8255.	8255.	8255.	8255.
39	Qout	-1.075E+04	-1.075E+04	5427.318	5427.044
40	Rd1	1.415735	0.4420096	1.415735	0.4672706
41	Rd2	0	0	1.006609	1.006609

42	Rd3	0	0	0.2764135	0.2764135
43	Rd4	0.404076	0.2342095	0.404076	0.2761825
44	rhoin	0.97	0.97	0.97	0.97
45	rhoout	0.88	0.88	0.88	0.88
46	Rp	8.225E+05	3.238E+04	8.225E+05	3.239E+04
47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	2.477E+04	2.477E+04	2.477E+04	2.477E+04

Table A.54: Polymath Result Standard Case CSTR 2

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	1.637123	0.8359641	1.637123	0.8375285
2	Ca0	1.637	1.637	1.637	1.637
3	Cc	1.636939	0.8358263	1.636939	0.8374042
4	Cc0	1.637	1.637	1.637	1.637
5	Cl	5.968245	5.968245	7.253944	7.253944
6	Cl0	5.968	5.968	5.968	5.968
7	Csb	6.142E-11	6.142E-11	5.009E-08	5.009E-08
8	Csb0	0	0	0	0
9	Cse	0.0002205	0.0002205	0.0003883	0.0003883
10	Cse0	0.0002206	0.0002206	0.0002206	0.0002206
11	Ct	9.242578	8.75799	9.242578	8.929349
12	Cw	0	0	0	0
13	Cw0	0	0	0	0
14	Cx	5.098E-05	5.098E-05	8.365E-05	8.365E-05
15	Cx0	5.1E-05	5.1E-05	5.1E-05	5.1E-05
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155
22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	1.209E+04	6576.499	1.209E+04	6576.499

25	kp0	94.24956	51.2831	94.24956	51.2831
26	mdotvent_co2	0.0121642	0.006539	0.0121642	0.0066081
27	mdotvent_nh3	0.0013219	0.0013219	0.0057401	0.0051054
28	mdotvent_w	583.6798	83.12024	583.6798	83.12024
29	na	2.665E+04	1.361E+04	2.665E+04	1.364E+04
30	nc	2.665E+04	1.361E+04	2.665E+04	1.363E+04
31	nco2	0	0	0	0
32	nl	9.717E+04	9.717E+04	1.181E+05	1.181E+05
33	nnh3	0	0	0	0
34	nsb	1.0E-06	1.0E-06	0.0008155	0.0008155
35	nse	3.59	3.59	6.321955	6.321955
36	nw	0	0	0	0
37	nx	0.83	0.83	1.361903	1.361903
38	Qin	5427.	5427.	5427.	5427.
39	Qout	4556.594	4556.594	5100.683	5100.683
40	Rd1	0.4672678	0.2385885	0.4672678	0.2390389
41	Rd2	1.006617	0.6912897	1.006617	0.6945232
42	Rd3	0.276397	0.14858	0.276397	0.1501497
43	Rd4	0.0388104	0.0388104	0.1685276	0.1498943
44	rhoin	0.88	0.88	0.88	0.88
45	rhoout	0.92	0.92	0.92	0.92
46	Rp	3.239E+04	4612.427	3.239E+04	4612.427
47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	1.628E+04	1.628E+04	1.628E+04	1.628E+04

Table A.55: Polymath Result Standard Case CSTR 3

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	0.8374828	0.5624562	0.8374828	0.5624939
2	Ca0	0.838	0.838	0.838	0.838
3	Cc	0.8373522	0.5613638	0.8373522	0.5613803
4	Cc0	0.837	0.837	0.837	0.837
5	Cl	7.25348	7.25348	7.663315	7.663315
6	Cl0	7.254	7.254	7.254	7.254
7	Csb	6.535E-11	6.535E-11	5.419E-08	5.419E-08
8	Csb0	0	0	0	0

9	Cse	0.0003882	0.0003882	0.0005124	0.0005124
10	Cse0	0.0003883	0.0003883	0.0003883	0.0003883
11	Ct	8.928787	8.769385	8.928787	8.787808
12	Cw	0	0	0	0
13	Cw0	0	0	0	0
14	Cx	8.364E-05	8.364E-05	0.000106	0.000106
15	Cx0	8.4E-05	8.4E-05	8.4E-05	8.4E-05
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155
22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	6576.504	4599.417	6576.504	4599.417
25	kp0	51.28314	35.86594	51.28314	35.86594
26	mdotvent_co2	0.0066075	0.0045652	0.0066075	0.0045701
27	mdotvent_nh3	0.0006961	0.0006961	0.0041061	0.0035276
28	mdotvent_w	83.11061	26.17463	83.11061	26.17463
29	na	1.282E+04	8607.267	1.282E+04	8607.845
30	nc	1.281E+04	8590.55	1.281E+04	8590.803
31	nco2	0	0	0	0
32	nl	1.11E+05	1.11E+05	1.173E+05	1.173E+05
33	nnh3	0	0	0	0
34	nsb	1.0E-06	1.0E-06	0.0008293	0.0008293
35	nse	5.94	5.94	7.840904	7.840904
36	nw	0	0	0	0
37	nx	1.28	1.28	1.622569	1.622569
38	Qin	5101.	5101.	5101.	5101.
39	Qout	4956.776	4956.776	5017.997	5017.997
40	Rd1	0.239024	0.1602425	0.239024	0.1602473
41	Rd2	0.6944838	0.5338911	0.6944838	0.5339836
42	Rd3	0.150137	0.1037308	0.150137	0.1038434
43	Rd4	0.0204369	0.0204369	0.1205556	0.1035714
44	rhoin	0.92	0.92	0.92	0.92
45	rhoout	0.93	0.93	0.93	0.93
46	Rp	4611.893	1452.372	4611.893	1452.372

47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	1.53E+04	1.53E+04	1.53E+04	1.53E+04

Table A.56: Polymath Result Standard Case CSTR 4

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	0.5625083	0.4326816	0.5625083	0.4326837
2	Ca0	0.562	0.562	0.562	0.562
3	Cc	0.561379	0.4315851	0.561379	0.4315875
4	Cc0	0.561	0.561	0.561	0.561
5	Cl	7.663279	7.663279	7.902559	7.902559
6	Cl0	7.663	7.663	7.663	7.663
7	Csb	6.643E-11	6.643E-11	5.744E-08	5.744E-08
8	Csb0	0	0	0	0
9	Cse	0.0005122	0.0005122	0.0006184	0.0006184
10	Cse0	0.0005124	0.0005124	0.0005124	0.0005124
11	Ct	8.787785	8.748799	8.787785	8.767572
12	Cw	0	0	0	0
13	Cw0	0	0	0	0
14	Cx	0.0001063	0.0001063	0.0001238	0.0001238
15	Cx0	0.000106	0.000106	0.000106	0.000106
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155
22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	4599.418	3630.276	4599.418	3630.276
25	kp0	35.86595	28.30865	35.86595	28.30865
26	mdotvent_co2	0.0045701	0.0035825	0.0045701	0.0035831
27	mdotvent_nh3	0.0004721	0.0004721	0.0031391	0.0027633
28	mdotvent_w	26.17524	12.21836	26.17524	12.21836
29	na	8468.	6513.588	8468.	6513.621
30	nc	8451.	6497.082	8451.	6497.118
31	nco2	0	0	0	0

32	nl	1.154E+05	1.154E+05	1.19E+05	1.19E+05
33	nnh3	0	0	0	0
34	nsb	1.0E-06	1.0E-06	0.0008647	0.0008647
35	nse	7.71	7.71	9.310079	9.310079
36	nw	0	0	0	0
37	nx	1.6	1.6	1.863772	1.863772
38	Qin	5018.	5018.	5018.	5018.
39	Qout	4936.766	4936.766	4951.612	4951.612
40	Rd1	0.1602469	0.1231969	0.1602469	0.1231976
41	Rd2	0.5339932	0.4492839	0.5339932	0.4492963
42	Rd3	0.1038416	0.0814014	0.1038416	0.0814147
43	Rd4	0.0138605	0.0138605	0.092164	0.0811303
44	rhoin	0.93	0.93	0.93	0.93
45	rhoout	0.94	0.94	0.94	0.94
46	Rp	1452.406	677.921	1452.406	677.921
47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	1.505E+04	1.505E+04	1.505E+04	1.505E+04

Table A.57: Polymath Result Standard Case CSTR 5

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	0.4326198	0.3555154	0.4326198	0.3555154
2	Ca0	0.433	0.433	0.433	0.433
3	Cc	0.4315428	0.3544409	0.4315428	0.3544409
4	Cc0	0.432	0.432	0.432	0.432
5	Cl	7.901925	7.901925	7.992964	7.992964
6	Cl0	7.903	7.903	7.903	7.903
7	Csb	6.731E-11	6.731E-11	5.957E-08	5.957E-08
8	Csb0	0	0	0	0
9	Cse	0.0006186	0.0006186	0.0007059	0.0007059
10	Cse0	0.0006184	0.0006184	0.0006184	0.0006184
11	Ct	8.76683	8.703764	8.76683	8.703765
12	Cw	0	0	0	0
13	Cw0	0	0	0	0

14	Cx	0.0001239	0.0001239	0.0001378	0.0001378
15	Cx0	0.000124	0.000124	0.000124	0.000124
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155
22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	3630.215	3068.038	3630.215	3068.038
25	kp0	28.30817	23.92435	28.30817	23.92435
26	mdotvent_co2	0.0035827	0.0029854	0.0035827	0.0029854
27	mdotvent_nh3	0.0003648	0.0003648	0.0025584	0.0023004
28	mdotvent_w	12.21508	6.968374	12.21508	6.968374
29	na	6427.	5281.537	6427.	5281.537
30	nc	6411.	5265.574	6411.	5265.574
31	nco2	0	0	0	0
32	nl	1.174E+05	1.174E+05	1.187E+05	1.187E+05
33	nnh3	0	0	0	0
34	nsb	1.0E-06	1.0E-06	0.000885	0.000885
35	nse	9.19	9.19	10.48756	10.48756
36	nw	0	0	0	0
37	nx	1.84	1.84	2.047834	2.047834
38	Qin	4952.	4952.	4952.	4952.
39	Qout	4939.001	4939.001	4944.581	4944.581
40	Rd1	0.1231848	0.1011759	0.1231848	0.1011759
41	Rd2	0.4492387	0.3949575	0.4492387	0.3949575
42	Rd3	0.0814054	0.0678343	0.0814054	0.0678352
43	Rd4	0.0107101	0.0107101	0.0751155	0.0675406
44	rhoin	0.94	0.94	0.94	0.94
45	rhoout	0.94	0.94	0.94	0.94
46	Rp	677.7392	386.601	677.7392	386.601
47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	1.486E+04	1.486E+04	1.486E+04	1.486E+04

Table A.58: Polymath Result Turndown Case CSTR 1

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	4.959501	1.35529	4.959501	1.443993
2	Ca0	5.	5.	5.	5.
3	Cc	4.959501	1.355227	4.959501	1.443753
4	Cc0	5.	5.	5.	5.
5	Cl	0	0	6.281815	6.281815
6	Cl0	0	0	0	0
7	Csb	6.027E-09	6.027E-09	4.748E-08	4.748E-08
8	Csb0	0	0	0	0
9	Cse	0	0	0.0003104	0.0003104
10	Cse0	0	0	0	0
11	Ct	9.919002	7.209734	9.919002	9.169942
12	Cw	0	0	0	0
13	Cw0	17.8	17.8	17.8	17.8
14	Cx	0	0	7.048E-05	7.048E-05
15	Cx0	0	0	0	0
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155
22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	3.344E+04	1.079E+04	3.344E+04	1.079E+04
25	kp0	260.7436	84.10993	260.7436	84.10993
26	mdotvent_co2	0	0	0.0111112	0.0111112
27	mdotvent_nh3	0.0155194	0.0071406	0.0155194	0.0085933
28	mdotvent_w	1.659E+04	2179.111	1.659E+04	2179.319
29	na	8.229E+04	2.249E+04	8.229E+04	2.396E+04
30	nc	8.229E+04	2.249E+04	8.229E+04	2.396E+04
31	nco2	0	0	0	0
32	nl	0	0	1.042E+05	1.042E+05
33	nnh3	0	0	0	0
34	nsb	0.0001	0.0001	0.0007878	0.0007878
35	nse	0	0	5.150374	5.150374
36	nw	0	0	0	0

37	nx	0	0	1.169482	1.169482
38	Qin	5531.	5531.	5531.	5531.
39	Qout	-1.262E+04	-1.262E+04	3579.709	3579.473
40	Rd1	1.4157	0.3868525	1.4157	0.4121225
41	Rd2	0	0	0.9514501	0.9514501
42	Rd3	0	0	0.25247	0.25247
43	Rd4	0.4556483	0.2096473	0.4556483	0.2523
44	rhoin	0.97	0.97	0.97	0.97
45	rhoout	0.89	0.89	0.89	0.89
46	Rp	8.225E+05	2.248E+04	8.225E+05	2.249E+04
47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	1.659E+04	1.659E+04	1.659E+04	1.659E+04

Table A.59: Polymath Result Turndown Case CSTR 2

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	1.444165	0.7038883	1.444165	0.7053849
2	Ca0	1.444	1.444	1.444	1.444
3	Cc	1.443979	0.7037129	1.443979	0.705218
4	Cc0	1.444	1.444	1.444	1.444
5	Cl	6.282667	6.282667	7.497307	7.497307
6	Cl0	6.282	6.282	6.282	6.282
7	Csb	9.314E-09	9.314E-09	5.57E-08	5.57E-08
8	Csb0	0	0	0	0
9	Cse	0.0003101	0.0003101	0.000535	0.000535
10	Cse0	0.0003104	0.0003104	0.0003104	0.0003104
11	Ct	9.171192	8.724261	9.171192	8.908558
12	Cw	0	0	0	0
13	Cw0	0	0	0	0
14	Cx	7.078E-05	7.078E-05	0.000113	0.000113
15	Cx0	7.0E-05	7.0E-05	7.0E-05	7.0E-05
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155

22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	1.079E+04	5609.809	1.079E+04	5609.809
25	kp0	84.11155	43.74491	84.11155	43.74491
26	mdotvent_co2	0.0111115	0.0056845	0.0111115	0.0057481
27	mdotvent_nh3	0.005272	0.004393	0.005272	0.0044421
28	mdotvent_w	405.3373	50.29024	405.3373	50.29024
29	na	1.551E+04	7557.649	1.551E+04	7573.717
30	nc	1.55E+04	7555.765	1.55E+04	7571.926
31	nco2	0	0	0	0
32	nl	6.746E+04	6.746E+04	8.05E+04	8.05E+04
33	nnh3	0	0	0	0
34	nsb	0.0001	0.0001	0.000598	0.000598
35	nse	3.33	3.33	5.744596	5.744596
36	nw	0	0	0	0
37	nx	0.76	0.76	1.213379	1.213379
38	Qin	3579.	3579.	3579.	3579.
39	Qout	2989.2	2989.2	3370.978	3370.978
40	Rd1	0.4121869	0.2008764	0.4121869	0.201306
41	Rd2	0.9515643	0.6188544	0.9515643	0.6219493
42	Rd3	0.2524761	0.1291648	0.2524761	0.130609
43	Rd4	0.1547868	0.128977	0.1547868	0.1304212
44	rhoin	0.89	0.89	0.89	0.89
45	rhoout	0.93	0.93	0.93	0.93
46	Rp	2.249E+04	2790.6	2.249E+04	2790.6
47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	1.074E+04	1.074E+04	1.074E+04	1.074E+04

Table A.60: Polymath Result Turndown Case CSTR 3

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	0.7123504	0.4692414	0.7123504	0.4692617
2	Ca0	0.712	0.712	0.712	0.712
3	Cc	0.7121527	0.4691087	0.7121527	0.469131
4	Cc0	0.712	0.712	0.712	0.712

5	Cl	7.667952	7.667952	8.042059	8.042059
6	Cl0	7.668	7.668	7.668	7.668
7	Csb	9.888E-09	9.888E-09	6.11E-08	6.11E-08
8	Csb0	0	0	0	0
9	Cse	0.000535	0.000535	0.0007008	0.0007008
10	Cse0	0.000535	0.000535	0.000535	0.000535
11	Ct	9.093103	8.959662	9.093103	8.981294
12	Cw	0	0	0	0
13	Cw0	0	0	0	0
14	Cx	0.0001127	0.0001127	0.0001416	0.0001416
15	Cx0	0.000113	0.000113	0.000113	0.000113
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155
22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	5554.002	3829.232	5554.002	3829.232
25	kp0	43.30973	29.86009	43.30973	29.86009
26	mdotvent_co2	0.0057929	0.0039212	0.0057929	0.0039254
27	mdotvent_nh3	0.0026544	0.0026544	0.0035263	0.003031
28	mdotvent_w	50.77605	15.19304	50.77605	15.19304
29	na	7204.	4745.438	7204.	4745.643
30	nc	7202.	4744.096	7202.	4744.322
31	nco2	0	0	0	0
32	nl	7.755E+04	7.755E+04	8.133E+04	8.133E+04
33	nnh3	0	0	0	0
34	nsb	0.0001	0.0001	0.0006179	0.0006179
35	nse	5.41	5.41	7.086876	7.086876
36	nw	0	0	0	0
37	nx	1.14	1.14	1.431839	1.431839
38	Qin	3371.	3371.	3371.	3371.
39	Qout	3281.112	3281.112	3318.968	3318.968
40	Rd1	0.2032855	0.1339081	0.2032855	0.1339145
41	Rd2	0.630463	0.4775516	0.630463	0.4776228
42	Rd3	0.1316268	0.0890987	0.1316268	0.0891926

43	Rd4	0.0779338	0.0779338	0.1035313	0.0889898
44	rhoin	0.93	0.93	0.93	0.93
45	rhoout	0.94	0.94	0.94	0.94
46	Rp	2817.558	842.9871	2817.558	842.9871
47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	1.011E+04	1.011E+04	1.011E+04	1.011E+04

Table A.61: Polymath Result Turndown Case CSTR 4

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	0.4692176	0.3551904	0.4692176	0.3551904
2	Ca0	0.469	0.469	0.469	0.469
3	Cc	0.4691172	0.3550812	0.4691172	0.3550812
4	Cc0	0.469	0.469	0.469	0.469
5	Cl	8.041981	8.041981	8.174538	8.174538
6	Cl0	8.042	8.042	8.042	8.042
7	Csb	1.004E-08	1.004E-08	6.407E-08	6.407E-08
8	Csb0	0	0	0	0
9	Cse	0.000701	0.000701	0.0008323	0.0008323
10	Cse0	0.0007008	0.0007008	0.0007008	0.0007008
11	Ct	8.981158	8.885805	8.981158	8.885805
12	Cw	0	0	0	0
13	Cw0	0	0	0	0
14	Cx	0.0001416	0.0001416	0.000163	0.000163
15	Cx0	0.000142	0.000142	0.000142	0.000142
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155
22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	3829.183	3017.637	3829.183	3017.637

25	kp0	29.85971	23.53133	29.85971	23.53133
26	mdotvent_co2	0.0039251	0.0030257	0.0039251	0.0030259
27	mdotvent_nh3	0.0017632	0.0017632	0.0026688	0.0023346
28	mdotvent_w	15.19097	6.860034	15.19097	6.860034
29	na	4672.	3536.631	4672.	3536.631
30	nc	4671.	3535.543	4671.	3535.543
31	nco2	0	0	0	0
32	nl	8.007E+04	8.007E+04	8.139E+04	8.139E+04
33	nnh3	0	0	0	0
34	nsb	0.0001	0.0001	0.000638	0.000638
35	nse	6.98	6.98	8.286958	8.286958
36	nw	0	0	0	0
37	nx	1.41	1.41	1.623096	1.623096
38	Qin	3319.	3319.	3319.	3319.
39	Qout	3302.833	3302.833	3311.696	3311.696
40	Rd1	0.1339105	0.1013587	0.1339105	0.1013587
41	Rd2	0.4775892	0.3976825	0.4775892	0.3976825
42	Rd3	0.0891875	0.0687492	0.0891875	0.0687556
43	Rd4	0.0517661	0.0517661	0.0783552	0.0685434
44	rhoin	0.94	0.94	0.94	0.94
45	rhoout	0.94	0.94	0.94	0.94
46	Rp	842.8723	380.5887	842.8723	380.5887
47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	9957.	9957.	9957.	9957.

Table A.62: Polymath Result Turndown Case CSTR 5

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Ca	0.3551731	0.2927361	0.3551731	0.2927363
2	Ca0	0.355	0.355	0.355	0.355
3	Cc	0.3550725	0.2926375	0.3550725	0.2926378
4	Cc0	0.355	0.355	0.355	0.355
5	Cl	8.173812	8.173812	8.338875	8.338875

6	Cl0	8.175	8.175	8.175	8.175
7	Csb	0	0	6.719E-08	6.719E-08
8	Csb0	0	0	0	0
9	Cse	0.0008323	0.0008323	0.0009581	0.0009581
10	Cse0	0.0008323	0.0008323	0.0008323	0.0008323
11	Ct	8.885053	8.885053	8.92539	8.92539
12	Cw	0	0	0	0
13	Cw0	0	0	0	0
14	Cx	0.000163	0.000163	0.0001824	0.0001824
15	Cx0	0.000163	0.000163	0.000163	0.000163
16	deltaH	-1932.284	-1932.284	-1932.284	-1932.284
17	K0	88.10242	88.10242	88.10242	88.10242
18	Kap	4.019E-189	4.019E-189	4.019E-189	4.019E-189
19	kd1	0.2854522	0.2854522	0.2854522	0.2854522
20	kd2	0.0136721	0.0136721	0.0136721	0.0136721
21	kd2c	0.8750155	0.8750155	0.8750155	0.8750155
22	kd3	0.4894293	0.4894293	0.4894293	0.4894293
23	kd4	53.46993	53.46993	53.46993	53.46993
24	kp	3017.796	2543.301	3017.796	2543.301
25	kp0	23.53257	19.83249	23.53257	19.83249
26	mdotvent_co2	0.0030258	0.002528	0.0030258	0.0025281
27	mdotvent_nh3	0	0	0.0021618	0.0019491
28	mdotvent_w	6.859893	3.927588	6.859893	3.927588
29	na	3529.	2908.625	3529.	2908.628
30	nc	3528.	2907.647	3528.	2907.649
31	nco2	0	0	0	0
32	nl	8.122E+04	8.122E+04	8.286E+04	8.286E+04
33	nnh3	0	0	0	0
34	nsb	0	0	0.0006676	0.0006676
35	nse	8.27	8.27	9.520091	9.520091
36	nw	0	0	0	0
37	nx	1.62	1.62	1.812586	1.812586
38	Qin	3312.	3312.	3312.	3312.
39	Qout	3269.913	3269.913	3272.998	3272.998
40	Rd1	0.1013562	0.083534	0.1013562	0.0835341
41	Rd2	0.3976575	0.3533232	0.3976575	0.3533265
42	Rd3	0.0687533	0.0574424	0.0687533	0.0574443
43	Rd4	0	0	0.0634697	0.0572244

44	rhoin	0.94	0.94	0.94	0.94
45	rhoout	0.95	0.95	0.95	0.95
46	Rp	380.5808	217.8736	380.5808	217.8736
47	T	601.15	601.15	601.15	601.15
48	t	0	0	50.	50.
49	tau	3.	3.	3.	3.
50	V	9936.	9936.	9936.	9936.

Additional Reactor Equations:

In addition to the results above, the product was analyzed using Equations A.23-25 to determine the average chain length and weight.

$$\varepsilon = \frac{\left(F_C^{liq}\right)_0 - F_C^{liq} - F_{SE}^{liq}}{\left(F_C^{liq}\right)_0} \qquad \textit{Equation A.47}$$

$$D_{Pn} = \frac{1+r}{1+r-2r\varepsilon} \qquad \textit{Equation A.48}$$

$$M_n = D_{Pn} M_o \qquad \textit{Equation A.49}$$

Where,

ε = the conversion of C groups

$(F_c^{liq})_0$ = the molar flow rate of C groups in the inlet

F_c^{liq} = the molar flow rate of C groups in the outlet

F_{SE}^{liq} = the molar flow rate of SE groups

r = the feed ratio of C groups to A groups

M_n = the number average molecular weight of the product

M_o = the molecular weight of a monomeric unit

D_{Pn} = the number average degree of polymerization of the product

The value of r was assumed to be one since equal amounts of HMDA and adipic acid were fed to the system, and none of the reactants exit the reactor through the vent in the model. Also, M_o is taken to be 113 amu. This was derived by dividing the molecular weight of a nylon 6,6 monomer (226 amu) by the number of amide links per monomer (2 links per monomer). The final number average molecular weight of the full capacity fiber product is 2635 amu. The final number average degree of polymerization is 23.3 monomers per molecule.

Section A.1 was based on *Simulation Model of Polyamide-6,6 Polymerization in a Continuous Two-Phase Flow Coiled Tubular Reactor* and *Process for making nylon 6,6* [18] [7].

A.2 Properties:

The specific heat of water and nylon polymer were calculated from the Equations A.26-27 [22].

$$C_{p_w} = 0.997092 + (3.96106 * 10^{-5})T - (5.4726 * 10^{-7})T^2 + (1.2037 * 10^{-8})T^3 \quad \textit{Equation A.50}$$

$$C_{p_{poly}} = \omega_w C_{p_w} + (1 - \omega_w)[0.4\varepsilon^2 + 0.5(1 - \varepsilon^2)] \quad \textit{Equation A.51}$$

Where,

C_{p_w} = the specific heat of water

T = the temperature in degrees Celsius

$C_{p_{poly}}$ = the specific heat of the nylon polymer solution

ω_w = the weight fraction of water

ε = the extent of reaction

The heat of vaporization of water at different temperatures was calculated using Equation A.28 [22].

$$\Delta H_{vap} = \frac{7724.74(T+273.15)^2}{((T+273.15)-45.15)^2} \quad \textit{Equation A.52}$$

Where,

ΔH_{vap} = the heat of vaporization of water in cal/mol

T = the temperature of water in degrees Celsius

The enthalpy of selected streams was calculated using Equation A.29.

$$h = \Delta H = \int_{T_{ref}}^{T} Cp_{poly}\, dT \quad \textit{Equation A.53}$$

Where,

h = the enthalpy of the stream

ΔH = the change in enthalpy from reference temperature

T = the temperature of the stream

T_{ref} = the reference temperature

Cp_{poly} = the specific heat of the nylon polymer solution

A.3 Reactor Design

<u>R-101 Design Calculation</u>

Using Equation 9:

$$V = v_0 * (\tau + t_{surge})$$

v_0 = 8.8651 m^3/hr, solved for assuming ideal mixture of water and HMDA inside R-101 and using the required mass flowrates and densities of HMDA and water.

τ = 30 minutes, estimated to create a well-mixed outlet stream

t_{surge} = 10 minutes, chosen to allow time for operator response

$$V_{R-101} = \left(8.8651 \frac{m^3}{hr}\right) * (30min + 10min) * (\frac{1\ hr}{60\ min})$$

$$V_{R-101} = 5.91\ m^3$$

<u>R-102 Design Calculation</u>

Using Equation 9:

$$V = v_0 * (\tau + t_{surge})$$

v_0 = 11.189 m^3/hr, solved for by summing the required mass flowrates of water, adipic acid and HMDA into R-102 and dividing by the density of the salt solution out using Equation 10-12.

τ = 45 minutes, determined based off literature

t_{surge} = 5 minutes, chosen to allow time for operator response

$$V_{R-102} = \left(11.189 \frac{m^3}{hr}\right) * (45min + 5min) * (\frac{1\ hr}{60\ min})$$

$$V_{R-102} = 9.32\ m^3$$

<u>R-103 Design Calculation</u>

Using Equation 9

$$V = v_0 * (\tau + t_{surge})$$

v_0 = 8.255 m^3/hr, solved for by using the mass flowrate out of E-104 and dividing by the density of the solution out using Equations 10-12

τ = 3 hours, determined based off literature

t_{surge} = 15 minutes, chosen to allow time for operator response

$$V_{R-103} = \left(8.255 \frac{m^3}{hr}\right) * (3\ hr + 15\ min * \left(\frac{1\ hr}{60\ min}\right))$$

$$V_{R-103} = 26.8\ m^3$$

R-104 Design Calculation

Using Equation 9:

$$V = v_0 * (\tau + t_{surge})$$

v_0 = 5.427 m^3/hr, obtained from the output the of polymerization reaction simulation done in Polymath

τ = 3 hours, determined based off literature

t_{surge} = 15 minutes, chosen to allow time for operator response

$$V_{R-104} = \left(5.427 \frac{m^3}{hr}\right) * (3\ hr + 15\ min * \left(\frac{1\ hr}{60\ min}\right))$$

$$V_{R-104} = 17.6\ m^3$$

R-105 Design Calculation

Using Equation 9:

$$V = v_0 * (\tau + t_{surge})$$

v_0 = 5.101 m^3/hr, obtained from the output the of polymerization reaction simulation done in Polymath

τ = 3 hours, determined based off literature

t_{surge} = 15 minutes, chosen to allow time for operator response

$$V_{R-105} = \left(5.101 \frac{m^3}{hr}\right) * (3\ hr + 15\ min * \left(\frac{1\ hr}{60\ min}\right))$$

$$V_{R-105} = 16.6\ m^3$$

R-106 Design Calculation

Using Equation 9:

$$V = v_0 * (\tau + t_{surge})$$

v_0 = 5.018 m^3/hr, obtained from the output the of polymerization reaction simulation done in Polymath

τ = 3 hours, determined based off literature

t_{surge} = 15 minutes, chosen to allow time for operator response

$$V_{R-106} = \left(5.018 \frac{m^3}{hr}\right) * (3\ hr + 15\ min * \left(\frac{1\ hr}{60\ min}\right))$$

$$V_{R-106} = 16.3\ m^3$$

R-107 Design Calculation

Using Equation 9:

$$V = v_0 * (\tau + t_{surge})$$

v_0 = 4.952 m^3/hr, obtained from the output the of polymerization reaction simulation done in Polymath

τ = 3 hours, determined based off literature

t_{surge} = 15 minutes, chosen to allow time for operator response

$$V_{R-107} = \left(4.952 \frac{m^3}{hr}\right) * (3\ hr + 15\ min * \left(\frac{1\ hr}{60\ min}\right))$$

$$V_{R-107} = 16.1\ m^3$$

A.4 Vessel Design

V-101 Design Calculation

Using Equation 13:

$$V = \frac{v_0 t_{holdup}}{\%_{normal\ fill}}$$

v_0 = 11.189 m^3/hr, solved for by using the mass flowrate out of R-102 and dividing by the density of the salt solution using Equation 10-12.

t_{holdup} = 5 minutes, based off of heuristic [31]

$\%_{normal\ fill}$ = 50%, chosen to have tank half-full at steady operation

$$V_{V-101} = \frac{\left(11.189 \frac{m^3}{hr}\right) * 5\ \mathrm{min}(\frac{1\ hr}{60\ min})}{50\%}$$

$$V_{V-101} = 1.865\ m^3$$

Then, using Equation 14:

$$D_{calc} = \left(\frac{V_{V-101} * 4}{\frac{L}{D} * \pi}\right)^{1/3}$$

$\frac{L}{D}$ = 3, based off heuristic [31]

$$D_{calc} = \left(\frac{(1.865\ m^3) * 4}{3 * \pi}\right)^{1/3}$$

$$D_{calc} = 0.925\ m$$

Rounding to the nearest 3 inches results in a diameter of 39 inches and converting back to meters results in an actual diameter of:

$$D_{actual} = .991\ m$$

Then, using Equation 15:

$$V_{actual} = \left(\frac{\frac{L}{D} * \pi}{4}\right) * (D_{actual})^3$$

$$V_{V-101,actual} = \left(\frac{3 * \pi}{4}\right) * (.991\ m)^3$$

$$V_{V-101,actual} = 2.29\ m^3$$

<u>V-102 Design Calculation</u>

Using Equation 13:

$$V = \frac{v_0 t_{holdup}}{\%_{normal\ fill}}$$

v_0 = 3.506 m^3/hr, solved for by using the mass flowrate out of E-102 and dividing by the density of the stream by using Equations 10-12.

t_{holdup} = 5 minutes, based off of heuristic [31]

$\%_{normal\ fill}$ = 50%, chosen to have tank half-full at steady operation

$$V_{V-102} = \frac{\left(3.506 \frac{m^3}{hr}\right) * 5 \min\left(\frac{1\ hr}{60\ min}\right)}{50\%}$$

$$V_{V-102} = 0.584\ m^3$$

Then, using Equation 14:

$$D_{calc} = \left(\frac{V_{V-102} * 4}{\frac{L}{D} * \pi}\right)^{1/3}$$

$\frac{L}{D}$ = 3, based off heuristic [31]

$$D_{calc} = \left(\frac{(0.584\ m^3) * 4}{3 * \pi}\right)^{1/3}$$

$$D_{calc} = 0.628\ m$$

Rounding to the nearest 3 inches results in a diameter of 27 inches and converting back to meters results in an actual diameter of:

$$D_{actual} = 0.686\ m$$

Then, using Equation 15:

$$V_{actual} = \left(\frac{\frac{L}{D} * \pi}{4}\right) * (D_{actual})^3$$

$$V_{V-102,actual} = \left(\frac{3 * \pi}{4}\right) * (0.686\ m)^3$$

$$V_{V-102,actual} = 0.760\ m^3$$

A.5 Heat Exchanger Design

The required heat transfer rate to a material in a heat-exchanger was calculated using the following equations:

$$\dot{Q} = \dot{m} * C_p * \Delta T \qquad \textit{Equation A.54}$$

$$\dot{Q} = \dot{m} * \Delta H_{vap} \qquad \textit{Equation A.55}$$

Where,

$\dot{Q}$ = the required heat transfer rate

$\dot{m}$ = the mass flowrate of the material in the heat-exchanger

C_p = the specific heat of the material in the heat-exchanger

ΔT = the change in temperature between the inlet and outlet conditions of the material

ΔH_{vap} = the heat of vaporization of the material in the heat-exchanger

The overall heat transfer coefficient in heat-exchangers was calculated using the following equation:

$$U_o = \left(\frac{D_o}{h_i D_i} + R''_{f,i}\frac{D_o}{D_i} + R''_w + R''_{f,o} + \frac{1}{h_o}\right)^{-1} \qquad \textit{Equation A.56}$$

Where,

U_o = the overall heat transfer coefficient

D_o = the outside diameter of the tubes

D_i = the inside diameter of the tubes

h_i = the heat transfer coefficient for the inside of the tubes

h_o = the heat transfer coefficient for the outside of the tubes

$R''_{f,i}$ = the fouling resistance inside the tubes

$R''_{f,o}$ = the fouling resistance outside the tubes

R_w'' = tube wall resistance

All shell-and-tube heat-exchangers were assumed to have an outer diameter of 0.75 inches, and inner diameter of 0.62 inches and a Birmingham Wire Gauge value of 16 in order to meet industry standards. The heat transfer coefficients, fouling resistances and tube wall resistances were obtained from tables found in literature [22] [8].

Table A.63: Overall Heat Transfer Coefficient Calculation Summary

Unit	E-101	E-102	E-103	E-105
tube-side	Water	CW	CW	Nylon 6,6 melt
shell-side	LPS	Steam	Water	CW
M.O.C	CS	SS	SS	SS
h_i Btu/(hr*ft^2*°F)	1000.00	1000.00	1000.00	39748.11 [5]
h_o Btu/(hr*ft^2*°F)	1500.00	1500.00	1000.00	1000.00
$R_{f,i}''$ (hr*ft^2*°F)/Btu	0.00	0.00	0.00	0.01
$R_{f,o}''$(hr*ft^2*°F)/Btu	0.00	0.00	0.00	0.00
R_w''(hr*ft^2*°F)/Btu	0.00	0.00	0.00	0.00
U_o Btu/(hr*ft^2*°F)	153.95	146.08	139.29	95.70

The correction factor of heat-exchangers was calculated using the following set of equations:

$$P = \frac{t_o - t_i}{T_i - t_i} \qquad \textit{Equation A.57}$$

$$R = \frac{T_i - T_o}{t_o - t_i} \qquad \textit{Equation A.58}$$

$$P' = \frac{1 - \left(\frac{1-PR}{1-P}\right)^{\frac{1}{n}}}{R - \left(\frac{1-PR}{1-P}\right)^{\frac{1}{n}}} \qquad \textit{Equation A.59}$$

$$F = \frac{\frac{\sqrt{R^2+1}}{R-1}\ln\left(\frac{1-P'}{1-P'R}\right)}{\ln\left(\frac{\frac{2}{P'}-1-R+\sqrt{R^2+1}}{\frac{2}{P'}-1-R-\sqrt{R^2+1}}\right)} \qquad \textit{EquationA. 60}$$

Where,

F = the correction factor

n = the number of shells

T_i = the hot stream inlet temperature

T_o = the hot stream outlet temperature

t_i = the cold stream inlet temperature

t_o = the cold stream outlet temperature

The log-mean temperature of heat-exchangers was calculated using the following equation:

$$\Delta T_{lm} = F * \frac{(T_i - t_o) - (T_o - t_i)}{\ln\left(\frac{T_i - t_o}{T_o - t_i}\right)} \qquad \textit{Equation A.61}$$

Where,

ΔT_{lm} = the log-mean temperature

F = the correction factor

T_i = the hot stream inlet temperature

T_o = the hot stream outlet temperature

t_i = the cold stream inlet temperature

t_o = the cold stream outlet temperature

Table A.64: Correction Factor and Log Mean Temperature Difference Calculation Summary

Unit	E-101	E-102	E-103	E-105
T_i (°F)	320	620.33	212	622.4
T_o (°F)	320	212	140	518
t_i (°F)	60	87	87	87
t_o (°F)	140	113	113	113
F	1	0.973179	0.9382	0.997938
ΔT_{lm} (°F)	214.0	272.9	73.6	469.1

<u>E-101 Design Calculation</u>
Using Equation 16:

$$A_0 = \frac{\dot{Q}}{U_o F \Delta T_{lm}}$$

$\dot{Q}$ = 956612 Btu/hr, calculated using Equation A.30 with the required mass flowrate of deionized water during startup condition (no water recycle stream) and the designed conditions of the inlet and outlet of E-101

U_o = 153.95 Btu/(hr*ft^2*°F), from Table A.11

F = 1, from Table A.12

ΔT_{lm} = 214.0 °F, from Table A.12

$$A_{0_{E-101}} = \frac{956612 \frac{Btu}{hr} * \frac{1\ m^2}{10.7639\ ft^2}}{\left(153.95 \frac{Btu}{hr * ft^2 * °F}\right) * 1 * 214.0°F}$$

$$A_{0_{E-101}} = 2.70\ m^2$$

E-102 Design Calculation
Using Equation 16:

$$A_0 = \frac{\dot{Q}}{U_o F \Delta T_{lm}}$$

$\dot{Q}$ = 8584070 Btu/hr, calculated using Equation A.30 to get the vent stream down to 212°F and then Equation A.31 to condense the vapor, both equations using the total mass flowrate of the vent streams off the polymerization reactors.

U_o = 146.07 Btu/(hr*ft^2*°F), from Table A.11

F = 0.973, from Table A.12

ΔT_{lm} = 272.9 °F, from Table A.12

$$A_{0_{E-102}} = \frac{8584070 \frac{Btu}{hr} * \frac{1\ m^2}{10.7639\ ft^2}}{\left(146.07 \frac{Btu}{hr * ft^2 * °F}\right) * 0.973 * 272.9°F}$$

$$A_{0_{E-102}} = 20.6\ m^2$$

E-103 Design Calculation
Using Equation 16:

$$A_0 = \frac{\dot{Q}}{U_o F \Delta T_{lm}}$$

$\dot{Q}$ = 534292 Btu/hr, calculated using Equation A.30 with the mass flowrate of the stream coming out of V-102 and the designed conditions of the inlet and outlet of E-103

U_o = 139.29 Btu/(hr*ft^2*°F), from Table A.11

F = 0.938, from Table A.12

ΔT_{lm} = 73.6 °F, from Table A.12

$$A_{0_{E-103}} = \frac{534292 \frac{Btu}{hr} * \frac{1\ m^2}{10.7639\ ft^2}}{\left(139.29 \frac{Btu}{hr * ft^2 * °F}\right) * 0.938 * 73.6°F}$$

$$A_{0_{E-103}} = 5.16\ m^2$$

<u>E-104 Design Calculation</u>

Using Equation 17:

$$A_0 = \frac{\dot{Q}}{U_0(T_{steam} - T_{bottoms})}$$

$\dot{Q}$ = 2163 kW, calculated using Equation 18 with the mass flowrates and enthalpies of the stream entering and leaving E-104.

U_0 = 2500 W/(m^2*°C), taken as the average of typical falling-film evaporator overall heat transfer coefficient values [17]

T_{steam} = 160°C, property of the low pressure steam

$T_{bottoms}$ = 143°C, determined from literature [18]

$$A_{0_{E-104}} = \frac{(2163\ kW)\frac{1000\ W}{1\ kW}}{(2500\frac{W}{m^2 * °C})(160°C - 143°C)}$$

$$A_{0_{E-104}} = 7.80\ m^2$$

<u>E-105 Design Calculation</u>

Using Equation 16:

$$A_0 = \frac{\dot{Q}}{U_o F \Delta T_{lm}}$$

$\dot{Q}$ = 438351 Btu/hr, calculated using Equation A.30 with the mass flowrate of the stream coming out of R-107 and the designed conditions of the inlet and outlet of E-105

U_o = 95.70 Btu/(hr*ft^2*°F), from Table A.11

F = 0.998, from Table A.12

ΔT_{lm} = 469.1 °F, from Table A.12

$$A_{0_{E-105}} = \frac{438351\frac{Btu}{hr} * \frac{1\ m^2}{10.7639\ ft^2}}{\left(95.70\frac{Btu}{hr * ft^2 * °F}\right) * 0.998 * 469.1°F}$$

$$A_{0_{E-105}} = 0.909\ m^2$$

A.6 Pump Design

The following equations were used to calculate the necessary change in pressure generated by the pumps in this process design:

$$\Delta P = P_{discharge} - P_{suction} \quad \textit{Equation A.62}$$

$$P_{suction} = P_1 + \rho_1 * g * h_1 - \Delta P_{line\ loss\ before\ pump} \quad \textit{Equation A.63}$$

$$P_{discharge} = P_2 + \rho_2 * g * h_2 + \Delta P_{line\ loss\ after\ pump} + \Delta P_{control\ valve} + \Delta P_{HEX} \quad \textit{Equation A.64}$$

Where,

ΔP = the change in pressure generated by the pump

$P_{discharge}$ = the pressure on the discharge side of the pump

$P_{suction}$ = the pressure on the suction side of the pump

P_1 = the pressure of the process unit that is the source of the stream

P_2 = the pressure of the process unit that is the destination of the stream

h_1 = the liquid height of the process unit that is the source of the stream

h_2 = the height of the process unit that is the destination of the stream

$\Delta P_{line\ loss\ before\ pump}$ = the sum of the line losses that occur before the pump

$\Delta P_{line\ loss\ after\ pump}$ = the sum of the line losses that occur after the pump

$\Delta P_{control\ valve}$ = the change in pressure due to control valves

ΔP_{HEX} = the change in pressure due to passing through a heat-exchanger

This design assume 100 ft. of piping before and after each pump, resulting in a change in pressure of 0.5 psi before the pump and 2.0 psi after the pump due to line losses. The change in pressure due to a single control valve was set to 7 psi. The change in pressure due to the stream passing through a heat-exchange was set to 6 psi. [31]

Table A.65: Pump Calculation Summary

Unit	$P_{suction}$ (psia)	$P_{discharge}$ (psia)	ΔP (psi)	Flow (gpm)	hyd hp
P-101	15.0	35.4	20.4	26.6	0.316
P-102	18.3	30.1	11.8	39.3	0.269
P-103	20.4	28.0	7.6	49.3	0.219
P-104	16.4	35.3	18.9	49.3	0.544
P-105	25.3	105.5	80.3	36.3	1.70
P-106	95.0	103.6	8.6	23.9	0.120
P-107	94.2	103.8	9.5	22.5	0.125
P-108	94.2	103.8	9.7	22.1	0.124

P-109	94.2	103.8	9.7	21.8	0.123
P-110	17.0	35.4	18.4	15.4	0.166

P-101 Design Calculation

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 0.316, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-101} = \frac{0.316}{0.35}$$

$$bhp_{P-101} = 0.903$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-101} = 1\ hp$$

P-102 Design Calculation

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 0.269, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-102} = \frac{0.269}{0.35}$$

$$bhp_{P-102} = 0.770$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-102} = 1\ hp$$

P-103 Design Calculation

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 0.219, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-103} = \frac{0.219}{0.35}$$

$$bhp_{P-103} = 0.625$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-103} = 0.75\ hp$$

P-104 Design Calculation

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 0.544, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-104} = \frac{0.544}{0.35}$$

$$bhp_{P-104} = 1.55$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-104} = 2\ hp$$

P-105 Design Calculation

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 1.70, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-105} = \frac{1.70}{0.35}$$

$$bhp_{P-105} = 4.86$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-105} = 5\ hp$$

P-106 Design Calculation

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 0.120, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-106} = \frac{0.120}{0.35}$$

$$bhp_{P-106} = 0.343$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-106} = 0.5\ hp$$

<u>P-107 Design Calculation</u>

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 0.125, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-107} = \frac{0.125}{0.35}$$

$$bhp_{P-107} = 0.357$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-107} = 0.5\ hp$$

<u>P-108 Design Calculation</u>

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 0.124, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-108} = \frac{0.124}{0.35}$$

$$bhp_{P-108} = 0.356$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-108} = 0.5\ hp$$

<u>P-109 Design Calculation</u>

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 0.123, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-109} = \frac{0.123}{0.35}$$

$$bhp_{P-109} = 0.351$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-109} = 0.5\ hp$$

<u>P-110 Design Calculation</u>

Using Equation 19:

$$bhp = \frac{hyd\ hp}{\varepsilon_{pump}}$$

$hyd\ hp$ = 0.166, from Table A.13

ε_{pump} = 0.35, graphically determined based on volumetric flowrate [9]

$$bhp_{P-110} = \frac{0.166}{0.35}$$

$$bhp_{P-110} = 0.473$$

Rounding up to the nearest available motor size gives a motor brakehorse power value of [9]:

$$bhp_{P-110} = 0.5\ hp$$

A.7 Furnace Design

The following equations were used to calculate the required heat transfer rate demanded by the polymerizations reactors.

$$\dot{Q}_{poly\ reactors} = \Delta H_{app} * \Delta C_{linkages} * V_{liquid} + \Delta H_{vap} * \dot{m}_{water\ vent} \qquad \textit{Equation A.65}$$

Where,

$\dot{Q}_{poly\ reactors}$ = the required heat transfer rate to polymerization reactor

ΔH_{app} = the heat of reaction of the polymerization reaction

$\Delta C_{linkages}$ = the change in the concentration of linkages from inlet to outlet of the reactor

V_{liquid} = the liquid volume of the reactor

ΔH_{vap} = the heat of vaporization of water

$\dot{m}_{water\ vent}$ = the mass flowrate of water being vented out of the reactor

x_w = the mole fraction of water

Since the assumption was made that there was no water in the nylon 6,6 melt mixture, the heat of reaction of the polymerization reaction remained a constant throughout all reactors. The change in concentration of linkages and mass flowrate of water being vented were obtained from the results of the Polymath simulation while the liquid volume was calculated from these results.

Table A.66: Polymerization Reactor Heat Transfer Rate Calculation Summary

Unit	R-103	R-104	R-105	R-106	R-107
ΔH_{app} (Btu/lbmol)	-0.831	-0.831	-0.831	-0.831	-0.831
$\Delta C_{linkages}$ (mol/L)	5.97	1.29	0.41	0.24	0.09
$\dot{m}_{water\ vent}$ (kg/hr)	3231.5	83.1	26.2	12.2	7.0
ΔH_{vap} (Btu/lbm)	901.7	901.7	901.7	901.7	901.7
$\dot{Q}_{poly\ reactors}$ (Btu/hr)	2790954	57556	18397	8025	6281

X-101 Design Calculation

Using Equation 21:

$$\dot{Q}_{furnace} = \sum \dot{Q}_{poly\ reactors}$$

$\dot{Q}_{R-103}$ = 2790000 Btu/hr, from Table A.14

$\dot{Q}_{R-104}$ = 57600 Btu/hr, from Table A.14

$\dot{Q}_{R-105}$ = 18400 Btu/hr, from Table A.14

$\dot{Q}_{R-106}$ = 8020 Btu/hr, from Table A.14

$\dot{Q}_{R-107}$ = 6280 Btu/hr, from Table A.14

$$\dot{Q}_{X-101} = (2790000 + 57600 + 18400 + 8020 + 6280)\frac{Btu}{hr} * \frac{0.000293\ kW}{\frac{Btu}{hr}}$$

$$\dot{Q}_{X-101} = 844\ kW$$

A.8 Conveyor Design

X-102 Design Calculation

Using Equation 22:

$$A = \frac{F}{belt\ speed}$$

F = 1.75 m^3/hr, calculated from the required mass of adipic acid into R-102 and the density of adipic acid

$belt\ speed$ = 150 m/hr, chosen to be slow enough to not kick up powder into the air

$$A_{X-102} = \frac{1.75\,\frac{m^3}{hr}}{150\,\frac{m}{hr}}$$

$$A_{X-102} = 0.0117\,m^2$$

<u>X-103 Design Calculation</u>

Using Equation 22:

$$A = \frac{F}{belt\ speed}$$

F = 2.83 m^3/hr, calculated from the required mass of HMDA into R-101 and the density of HMDA

$belt\ speed$ = 150 m/hr, chosen to be slow enough to not kick up powder into the air

$$A_{X-102} = \frac{2.83\,\frac{m^3}{hr}}{150\,\frac{m}{hr}}$$

$$A_{X-102} = 0.0189\,m^2$$

A.9 Economic Analysis

Capital Costs

The free on board, FOB, vanilla purchase price was calculated for each piece of equipment using Equation A.42.

$$log_{10}\left(C_p^o\right) = K_1 + K_2 log_{10}(A) + K_3[log_{10}(A)]^2 \qquad \textit{Equation A.66}$$

Where,

C_p^o = FOB vanilla purchase price

A = Capacity of the size parameter

K_n = FOB purchase cost coefficients from Table A.1 in Turton [31].

The values of the FOB purchase cost coefficients are summarized in Table A.15.

The FOB vanilla purchase cost was calculated using a costing correlation from 2001. To determine the FOB vanilla purchase cost of equipment in 2017, the 2001 value was multiplied by the mid-2016 CEPCI value and divided by the 2001 CECPI value.

$$F_{BM} = B_1 + B_2 F_M F_P \qquad \textit{Equation A.67}$$

Where,

F_{BM} = Bare Module Factor

F_M = Material Factor

F_P = Pressure Factor

B_1 and B_2 are coefficients that vary with the type of equipment that were taken from Table A.4 in Turton [31]. The bare module factor for the majority of the equipment was calculated using Equation A.43. The bare module factors of the jacketed agitated reactors, the mixer/settler, and the apron conveyors were taken from Table A.7 in Turton [31] rather than calculated using Equations A.41-43. The bare module factors of the nonreactive fired heater and the falling film evaporator were similarly taken from Figure A.19 and Table A.6 in Turton [31].

$$C_{BM} = F_{BM} C_p^o \qquad \textit{Equation A.68}$$

$$C_{BM} = F_{BM} C_p^o F_P \qquad \textit{Equation A.69}$$

Where,

C_{BM} = Bare Module Cost

F_{BM} = Bare Module Factor

C_p^o = FOB vanilla purchase price

F_P = Pressure Factor

The bare module cost of the nonreactive fired heater and the falling film evaporator was calculated using Equation A.45. The bare module cost of the remainder of the process equipment was calculated using Equation A.44.

$$F_P = \frac{\frac{(P+1)D}{2[850-0.6(P+1)]}+0.00315}{0.0063} \qquad \textit{Equation A.70}$$

$$log_{10}(F_P) = C_1 + C_2 log_{10}(P) + C_3[log_{10}(P)]^2 \qquad \textit{Equation A.71}$$

Where,

P = Design Pressure (barg)

D = Process Vessel Diameter (m)

C_n = Pressure factor coefficients from Table A.2 in Turton [31]

The values of the pressure factor coefficients are summarized in Table A.15.

The material factor for each piece of equipment was found on Table A.3 and Figure A.18 in Turton [31]. The pressure factors were calculated using a design pressure 50psi greater than the maximum operating pressure. The pressure factor for V-101 and V-102 were both calculated to be less than 1 using Equation A.46. The bare module cost for the vessels was then calculated using a pressure factor of 1. The pressure factor for the remaining pieces of equipment was determined using Equation A.47. A pressure factor of 1 was used if the design pressure was less than the range of pressures listed in Table A.2 of Turton [31].

$$C_{GR} = 1.18 C_{BM} + 0.5 C_{BM}^o \qquad \textit{Equation A.72}$$

Where,

C_{GR} = Grassroots Cost

C_{BM} = Bare Module Cost

C_{BM}^{o} = Vanilla Bare Module Cost

Since this project calls for grassroots design, the grassroots cost was used as the total installed cost. The grassroots cost was calculated using Equation A.48. The vanilla bare module cost was calculated the same way as the bare module cost using a material and pressure factor of 1. The factor 1.18 accounts for contingency costs and fees. The vanilla bare module cost term accounts for the cost of site and utility development.

Table A.15 contains a summary of the size parameters, FOB purchase cost coefficients, and the pressure factor coefficients of the process equipment.

Table A.67: Capital Costing Factors and Coefficients Summary

	K_1	K_2	K_3	A	C_1	C_2	C_3	B_1	B_2
Mixer/Settler	4.7116	0.4479	0.0004	Volume (m^3)	NA	NA	NA	NA	NA
Jacketed Agitated Reactor	4.1052	0.53	-0.0005	Volume (m^3)	NA	NA	NA	NA	NA
Centrifugal Pump (P>10barg)	3.3892	0.0536	0.1538	Shaft Power (kW)	-0.3935	0.3957	-0.00226	1.89	1.35
Fixed Tube Heat Exchanger (Shell and Tube P>5barg)	4.3247	-0.303	0.1634	Area (m^2)	0.03881	-0.11272	0.08183	1.63	1.66
Falling Film Evaporator (P>10barg)	3.9119	0.8627	-0.0088	Area (m^2)	0.1578	-0.2992	0.1413	NA	NA
Horizontal Process Vessels	3.5565	0.3776	0.0905	Volume (m^3)	NA	NA	NA	1.49	1.52
Nonreactive Fired Heater	7.3488	-1.1666	0.2028	Duty (kW)	0.1347	-0.2368	0.1021	NA	NA

Cost of Manufacturing

The cost of manufacturing (COMd) was calculated using the equation developed on Table A.16. The developed equations for the direct, fixed, and general manufacturing costs were also calculated using the equations developed on Table A.16. The variables used to calculate the COMd are summarized on Table A.17.

The cost of utilities was calculated by multiplying the utility requirements by the price of the utilities found on Table 8.3 in Turton [31]. The cost of waste treatment was calculated by multiplying the liquid flowrate of the waste water by the cost of primary waste water treatment found on Table 8.3 in Turton [31].

The cost of raw materials was calculated by multiplying the required amounts of HMDA, adipic acid, and deionized water by their respective costs. The HMDA and adipic acid prices, $2,500 and $1,200 per metric ton respectively, are taken from an Invista quote [13]. The price of deionized water was taken from Table 8.3 in Turton [31]. The required amount of deionized water was calculated while taking the recycle water stream into account.

The cost of operating labor was calculated using the annual mean wage of chemical plant and system operators in the West Kentucky nonmetropolitan area, $63,920 [2]. The number of operators required per shift for each design was calculated using Equation A.49.

$$N_{OL} = (6.29 + 31.7P^2 + .23N_{np})^{0.5} \qquad \textit{Equation A.73}$$

Where,

N_{OL} = Number of operators required per shift

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

N_{np} = Number of compressors, towers, reactors, heaters, and exchangers

The handling of HMDA and adipic acid results in two processing steps involving the handling of particulate solids. This greatly increases the number of required operators. The extruders were also included in the calculation of N_{np} as it was decided that the yarn extruders in particular would require as much if not more attention than a reactor or heat exchanger. All of the equipment excluding the pumps, process vessels, and conveyors were included in the N_{np} calculation to obtain a conservative estimate of the required number of operators [31].

The total number of operators required was 4.5 times the number of operators required for each shift, rounded up. The total number of operators was each paid a wage of $63,920 which resulted in the annual cost of operating labor.

Table A.68: Cost of Manufacturing Factors

1	**Direct Manufacturing Costs**	Typical Range of Multiplying Factors	Value Used in Design
a	Raw Materials	CRM	CRM
b	Waste Treatment	CWT	CWT
c	Utilities	CUT	CUT
d	Operating Labor	COL	COL

e	Direct Supervisory and clerical labor	(0.1-0.25)COL	0.18COL
f	Maintenance and repairs	(0.02-0.1)FCI	0.06FCI
g	Operating Supplies	(0.1-0.2)(Line 1.F)	0.009FCI
h	Laboratory Charges	(0.1-0.2)COL	0.15COL
i	Patents and Royalties	(0-0.06)COM	0.03COM
Total Direct Manufacturing Costs		CRM+CWT+CUT+1.33COL+0.03COM+0.069FCI	
2	**Fixed Manufacturing Costs**	Typical Range of Multiplying Factors	Value Used in Design
a	Depreciation	0.1FCI	*0
b	Local Taxes and Insurance	(0.014-0.05)FCI	0.032FCI
c	Plant Overhead Costs	(0.50-0.7)(Line 1.D + Line 1.E + Line 1.F)	0.708COL+0.036FCI
Total Fixed Manufacturing Costs		0.708COL+0.068FCI	
3	**General Manufacturing Expenses**	Typical Range of Multiplying Factors	Value Used in Design
a	Administration Costs	(0.50-0.7)(Line 1.D + Line 1.E + Line 1.F)	0.177COL+0.009FCI
b	Distribution and Selling Costs	(0.02-0.2)COM	0.11COM
c	Research and Development	0.05COM	0.05COM
Total General Manufacturing Costs		0.177COL+0.009FCI+0.16COM	
Total Costs		CRM+CWT+CUT+2.215COL+0.16COM+0.146FCI	
COMd		0.180FCI+2.73COL+1.23(CRM+CWT+CUT)	

Table A.69: Manufacturing Costs

	Full Nylon 6,6 Fiber Production	Full Granular Nylon 6,6 Production	Turndown Nylon 6,6 Fiber Production
Total Installed Cost (FCI):	$ 15,349,728	$ 8,653,442	$ 15,349,728
Cost of Operating Labor (COL):	$ 3,707,360	$ 3,387,760	$ 3,707,360
Cost of Utilities (CUT):	$ 1,912,003	$ 1,291,847	$ 1,504,027
Cost of Raw Materials (CRM):	$ 91,535,135	$ 91,535,135	$ 61,328,333
Cost of Waste Treatment (CWT)	$ 1,156	$ 1,156	$ 774
Direct Manufacturing Costs:	$ 103,286,404	$ 101,693,739	$ 71,537,351
Fixed Manufacturing Costs:	$ 3,668,592	$ 2,986,968	$ 3,668,592
General Manufacturing Costs:	$ 21,318,035	$ 20,745,747	$ 15,270,597
Cost of Manufacturing (COMd)	$ 128,273,032	$ 125,426,455	$ 90,476,540
Total Costs	$ 128,273,032	$ 125,426,455	$ 90,476,540

Payback Period, NPV, and DCFROR Analysis

The production rate was specified in the design statement [20]. The nylon 6,6 fiber sale price was calculated using the average price per kilogram of nylon yarn tabulated in 2016 under the commodity codes 540241, 540245, 540251, and 540261 [32]. The sum of the annual trade was divided by the sum of the net weight to determine the average price. Only entries with a nonzero net weight were considered. The price of nylon 6,6 granules was taken from literature [10]. The sales revenue was calculated by multiplying the annual production by the sales price.

The depreciation was calculated using MACRS depreciation. The recovery period was 10 years and the half year convention was used [14]. Undiscounted book value and working capital were depreciated in the final year. The MACRS depreciation rate was multiplied by the fixed capital investment to calculate the depreciation for each year. The depreciation and cost of manufacturing were subtracted from the net revenue to obtain the taxable income for each year. The other operating cost value is the difference between the sum of the CRM, CUT, COL, and CWT and the COMd.

The cost of manufacturing for each case was calculated using the values summarized in Table A.17 and the equations summarized in Table A.16. The direct, fixed, and general manufacturing costs were calculated similarly.

The tax is calculated by multiplying the taxable income by -40%. The net income is the sum of the taxable income and tax lines. This project would likely be considered by a company large enough to justify using expense taxes meaning that if the taxable income is ever negative, the tax benefits can be realized immediately of other company projects. The depreciation is added to the net income and the fixed and working capital are subtracted from the net income to obtain the undiscounted cash flow for each year. The working capital was estimated to be 5% of the fixed capital and is acquired in 2018 during startup [31]. The discounted cash flow is the product of the cash flow and the discount factor. The discount factor, $P/F_{i,n}$, is calculated using the hurdle rate and the number of years past the start of the project evaluation lifetime.

The DCFROR is calculated by using the IRR Excel function with the undiscounted cash flow serving as the entries. The NPV is calculated as the sum of the discounted cash flow. The cost of manufacturing per pound of nylon 6,6 produced is calculated by dividing the COMd by the production rate. To calculate the discounted payback period, the first year with a positive NPV is found. This is done by summing the discounted cash flow of an increasing amount of years, until the result is positive. The discounted payback period lies between these two years. The exact discounted payback period is calculated by adding the number of year when the NPV was last negative to the absolute value of the final negative NPV divided by the discounted cash flow of the subsequent year. The undiscounted payback period is calculated similarly, but utilizing the undiscounted cash flow [28].

Sensitivity Analysis

Two cash flow tables were constructed for each variable incorporated into the tornado charts. One of these tables featured the high end of the variable range, while the other was calculated with the lowest value in the range of variation. The cash flow tables were calculated in exactly the same manner the 3 main tables were. The range of variations tested can be found on Table 52 and the results of the sensitivity analysis are summarized in Figure 4.

Table A.70: Example Cash Flow Table

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
Nylon 66 Production (lbm/year)		85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000	85,000,000
Nylon 66 Sales Price	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24	2.24
Sales Revenue	-	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062
+ Salvage Value											
- Royalties											
Net Revenue	-	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062	190,181,062
-Raw Materials		(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)	(91,535,135)
-Utilities		(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)	(1,912,003)
-Operating Labor		(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)	(3,707,360)
-Waste Treatment		(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)	(1,156)
- Other Op Costs		(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)	(31,117,379)
- Depreciation		(1,534,973)	(2,762,951)	(2,210,361)	(1,768,289)	(1,415,245)	(1,131,275)	(1,005,407)	(1,005,407)	(1,006,942)	(1,005,407)
- Amortization											
- Depletion											
- Loss Forward											
- Writeoff											(1,270,958)
Taxable Income	-	60,373,058	59,145,080	59,697,670	60,139,742	60,492,786	60,776,756	60,902,623	60,902,623	60,901,088	59,631,666
- Tax @40%	-	(24,149,223)	(23,658,032)	(23,879,068)	(24,055,897)	(24,197,114)	(24,310,702)	(24,361,049)	(24,361,049)	(24,360,435)	(23,852,666)
Net Income	-	36,223,835	35,487,048	35,818,602	36,083,845	36,295,671	36,466,053	36,541,574	36,541,574	36,540,653	35,779,000
+ Depreciation	-	1,534,973	2,762,951	2,210,361	1,768,289	1,415,245	1,131,275	1,005,407	1,005,407	1,006,942	1,005,407
+ Amortization	-	-	-	-	-	-	-	-	-	-	-
+ Depletion	-	-	-	-	-	-	-	-	-	-	-
+ Loss Forward	-	-	-	-	-	-	-	-	-	-	-
+ Writeoff	-	-	-	-	-	-	-	-	-	-	1,270,958
- Working Capital		(767,486)									
- Fixed Capital	(15,349,728)										
Cash Flow	(15,349,728)	36,991,321	38,249,999	38,028,963	37,852,134	37,710,916	37,597,328	37,546,981	37,546,981	37,547,595	38,055,364
Discount factor (P/Fi,n)	1.000	0.870	0.756	0.658	0.572	0.497	0.432	0.376	0.327	0.284	0.247
Discounted Cash Flow	(15,349,728)	32,166,366	28,922,494	25,004,660	21,642,080	18,748,990	16,254,363	14,115,301	12,274,175	10,673,370	9,406,704
NPV @ i* =	173,858,776										
DCFROR =	243%										

Total Installed Cost (FCI):	$ 15,349,728
Cost of Operating Labor (COL):	$ 3,707,360
Cost of Utilities (CUT):	$ 1,912,003
Cost of Raw Materials (CRM):	$ 91,535,135
Cost of Waste Treatment (CWT)	$ 1,156
Direct Manufacturing Costs:	$ 103,286,404
Fixed Manufacturing Costs:	$ 3,668,592
General Manufacturing Costs:	$ 21,318,035
Cost of Manufacturing (COMd)	$ 128,273,032
Total Costs	$ 128,273,032

	Years	Months
Undiscounted Payback Period	0.41	5
Discounted Payback Period	0.48	6

	Year	0	1
Undiscounted	NPV @ i=0	(15,349,728)	16,816,638

	Year	0	1
Discounted	NPV @ i=i*	(15,349,728)	21,641,593

Table A.71: Time Log (hours)

	Person 1	Person 2	Person 3	Person 4
7-Feb				
8-Feb	2	2	2	2
9-Feb				
10-Feb				
11-Feb	3.5	2.5	3.5	2.5
12-Feb	2.5	2.5	2.5	2.5
13-Feb	3.5	3.5	3	3.5
14-Feb				
15-Feb	2	2	2	2
16-Feb				
17-Feb	3	3	3	3
18-Feb				
19-Feb	2.5	2.5	2.5	2.5
20-Feb	3	3.5	3.5	3.5
21-Feb	4	4	4	3.5
22-Feb	2.5	2.5	2.5	2.5
23-Feb		1.5		
24-Feb	4.5	4	4	4
25-Feb	3.5	3.5	3.5	3.5
26-Feb	4	3.5	3	3.5
27-Feb				
28-Feb	5	5.5	0.5	5.5
1-Mar	4.5	5	5	5
2-Mar	3	3	3	3
3-Mar	3	4	3	3
4-Mar	3	8	3	8
5-Mar	6	12	6	13
6-Mar	8	7	8	7
7-Mar	11	13	12	12
8-Mar	1			
9-Mar				