MEMORANDUM

Date: 9 March 2017

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

From Group 4287: Michele Higgins
Ryan Neal
Noah Gade
Rebecca Eastwood

Subject: Manufacturing Facility for Nylon-6,6

This memorandum is in response to the proposed manufacturing facility for nylon-6,6 for the AIChE 2017 Student Design Competition. The group was tasked with preparing a complete economic analysis of building a grass roots plant in the Calvert City, Kentucky area to produce 85MM pounds per year of nylon-6,6 from adipic acid and hexamethylenediamine. Byproduct streams of the process, changes in manufacturing output due to market conditions, control strategies, and safety and environmental factors were all considered in the analysis.

This report outlines the processes investigated as well as the economic evaluations of those processes. An appendix with detailed supporting figures and tables about the design methods and evaluation techniques is also included.

If you have any questions, feel free to contact us.

Sincerely,

Group 4287

Manufacturing Facility for Nylon-6,6

Group 4287

9 March 2017

Table of Contents

List of Tables and Figures

Abstract

The purpose of this project is to evaluate the feasibility of constructing a nylon-6,6 plant from grassroots in Calvert City, Kentucky. While designing, evaluating, and optimizing the production process of nylon-6,6, there were several conclusions that were drawn. These conclusions include: a continuous design is economically superior in comparison to a batch design, it is economically attractive to move forward with this project into the detailed design phase, and the control system proposed is a foundation that can be built upon in the later stages of design. The simplified control system decreases inherent safety concerns present in the production process and mitigates the overall risk associated with the formation of nylon-6,6. The economic conclusion is solidified by the growing nylon-6,6 market, and steady demand for the product. Additionally, it was determined that delivering a pelletized product, rather than a spun fiber, would allow the plant to appeal to a broader customer regime. This versatile product ensures long-term positive revenue generation from the proposed design.

Introduction

The objective of this project is to design a manufacturing facility that produces nylon-6,6 via the polycondensation of hexamethylenediamine (HMDA) and adipic acid (ADA)[47]. Industrial production of nylon-6,6 is potentially profitable due to its use in fiber applications as well as engineering thermoplastics. The synthesis uses equimolar amounts of HMDA and ADA; which are combined with water in a mixer to make a nylon salt solution[47]. The salt solution then polymerizes with the removal of water in reactors and is further condensed in flash tanks to form molten nylon-6,6[47]. The nylon product can then be spun into fibers through spinnerets and cooled or extruded and granulated into pellets. The two most commonly used industrial processes to produce nylon are a batch or a continuous system.

To accurately determine the superior design, both types of processes were simulated and evaluated. The batch process allows for better control of the process specifications, but the continuous process streamlines the production of nylon-6,6. Batch processes typically have a higher degree of industrial hygiene; however, the continuous process is less labor intensive to operate. These two design options were analyzed economically through NPV, sensitivity, and payback period. Additionally, safety, health, and environmental considerations were evaluated through a preliminary hazard analysis.

The manufacturing process has a side product stream of nitrous oxide. There is some nitrous oxide present in the ADA that is purchased and put into the process[39]. Although the supplier removes most of the nitrous oxide, a remaining small fraction will enter the process and contaminate the water product[60]. This water stream will be sent to a nitrous oxide scrubber, which converts the nitrous oxide to nitrogen gas via contact with a low NOx burner.

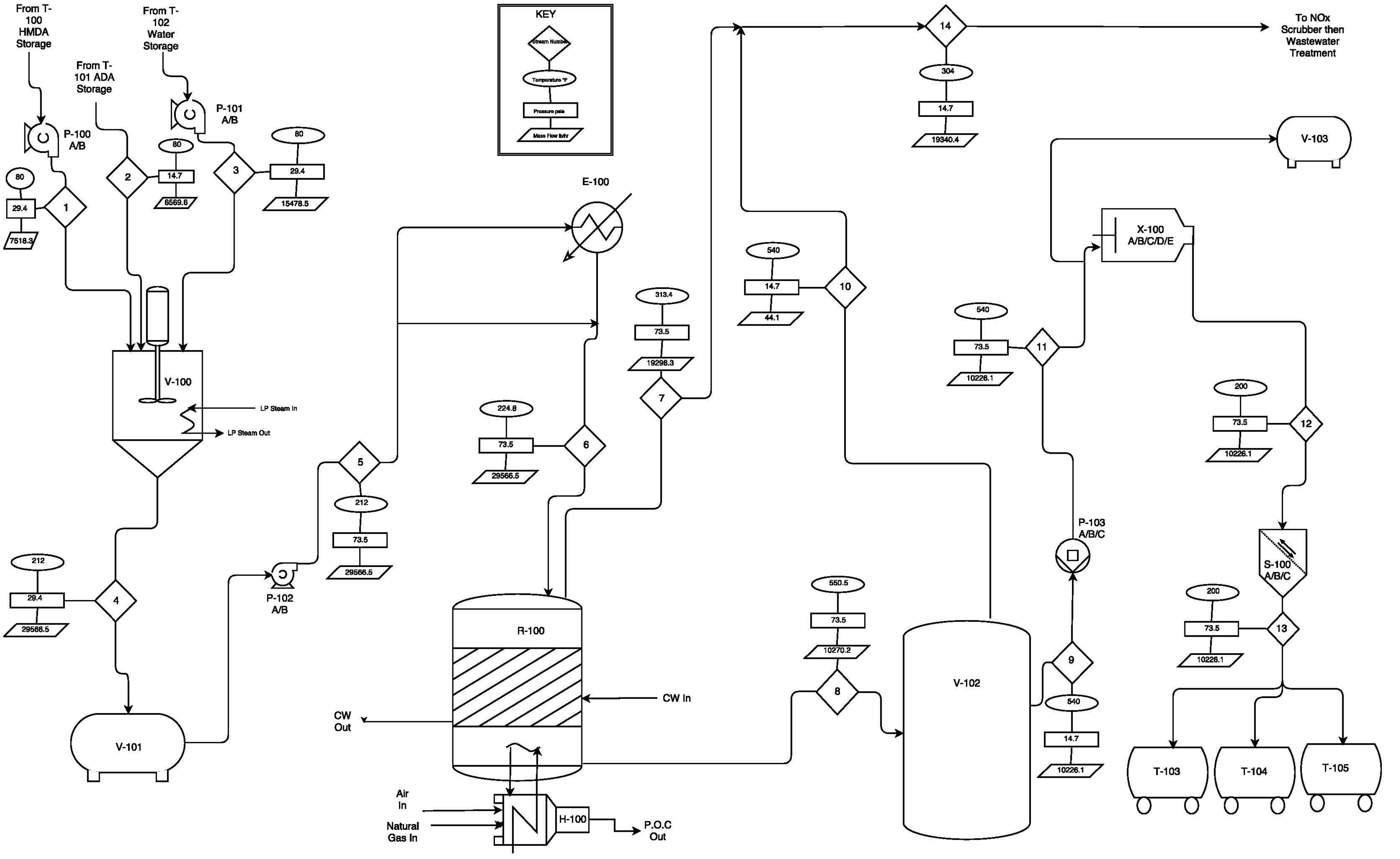
Due to potential changes in demand for nylon-6,6 production, the process will have to have the capability to operate at a reduced capacity of 67% . This will lessen the burden of storing large amounts of the product onsite when demand decreases. However, to determine if the designed pumps can handle the change in capacity pump curves would have to be evaluated. This was deemed to be outside of the preliminary design scope.

The remainder of this report will outline the methods used to complete the preliminary design for the nylon-6,6 production process. The report will discuss the simulation methods, economic analyses, hazard identification, final conclusions, and recommendations that the group has determined for the process.

Process Flow Diagram and Material Balances

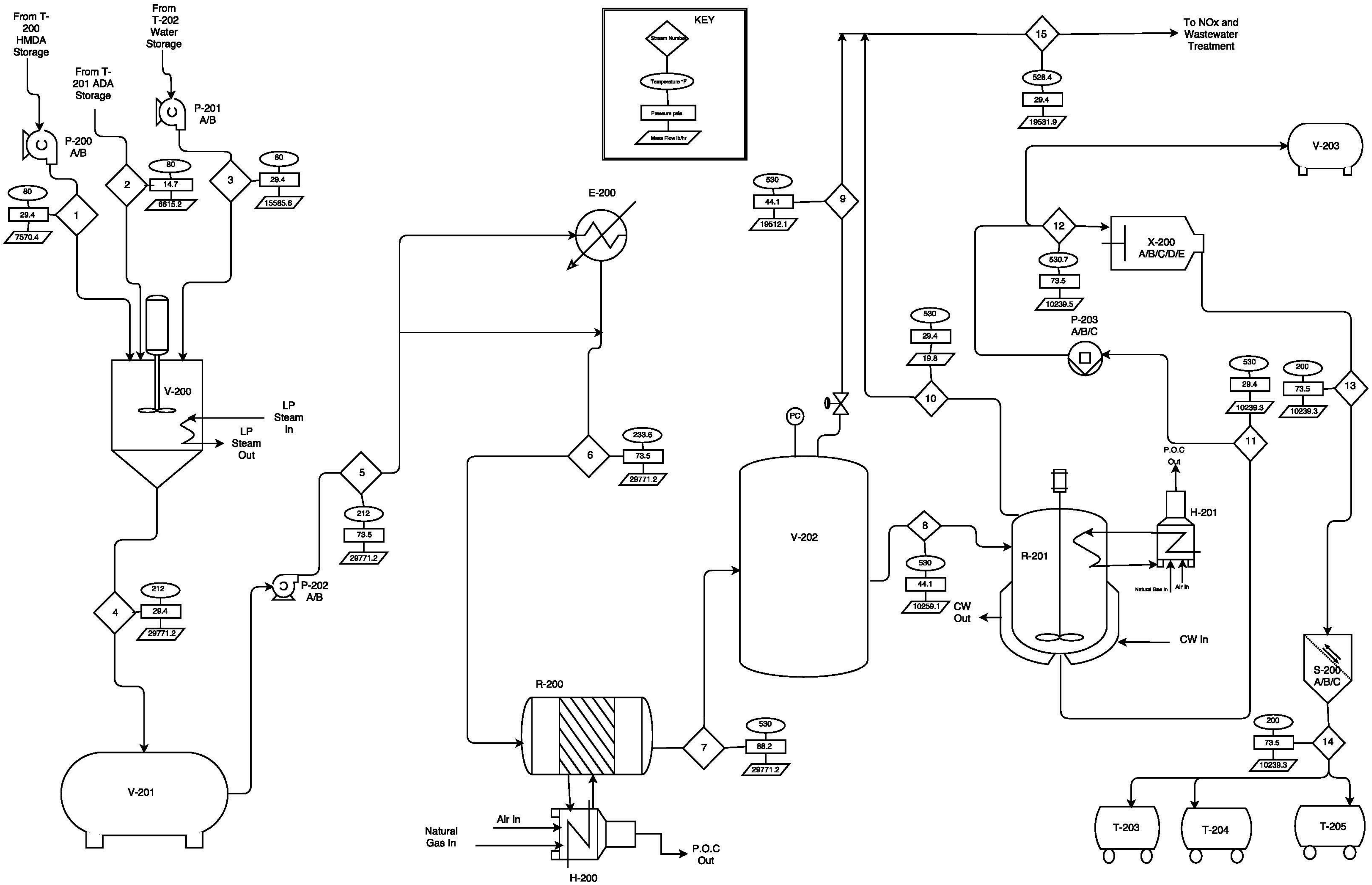
Process Flow Diagram

As mentioned, the group investigated two separate processes for the nylon-6,6 production from HMDA and ADA. The group has designed both processes and compared them economically. Process flow diagrams for the batch (Figure 1) and continuous processes (Figure 2) are shown on the following pages.



Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Stream Description	HMDA Flow into V-100	ADA Flow into V-100	Water Flow into V-100	Nylon Salt Flow from V-100	Nylon Salt Flow from V-101	Nylon Salt flow to R-100	Vapor Flow from R-100	Flow to V-102	Flow to P-103 A/B	Vapor Flow from V-102	Flow to X-100	Flow to S-101	Flow to Nylon-6,6 Storage	Flow to N_2O Scrubber

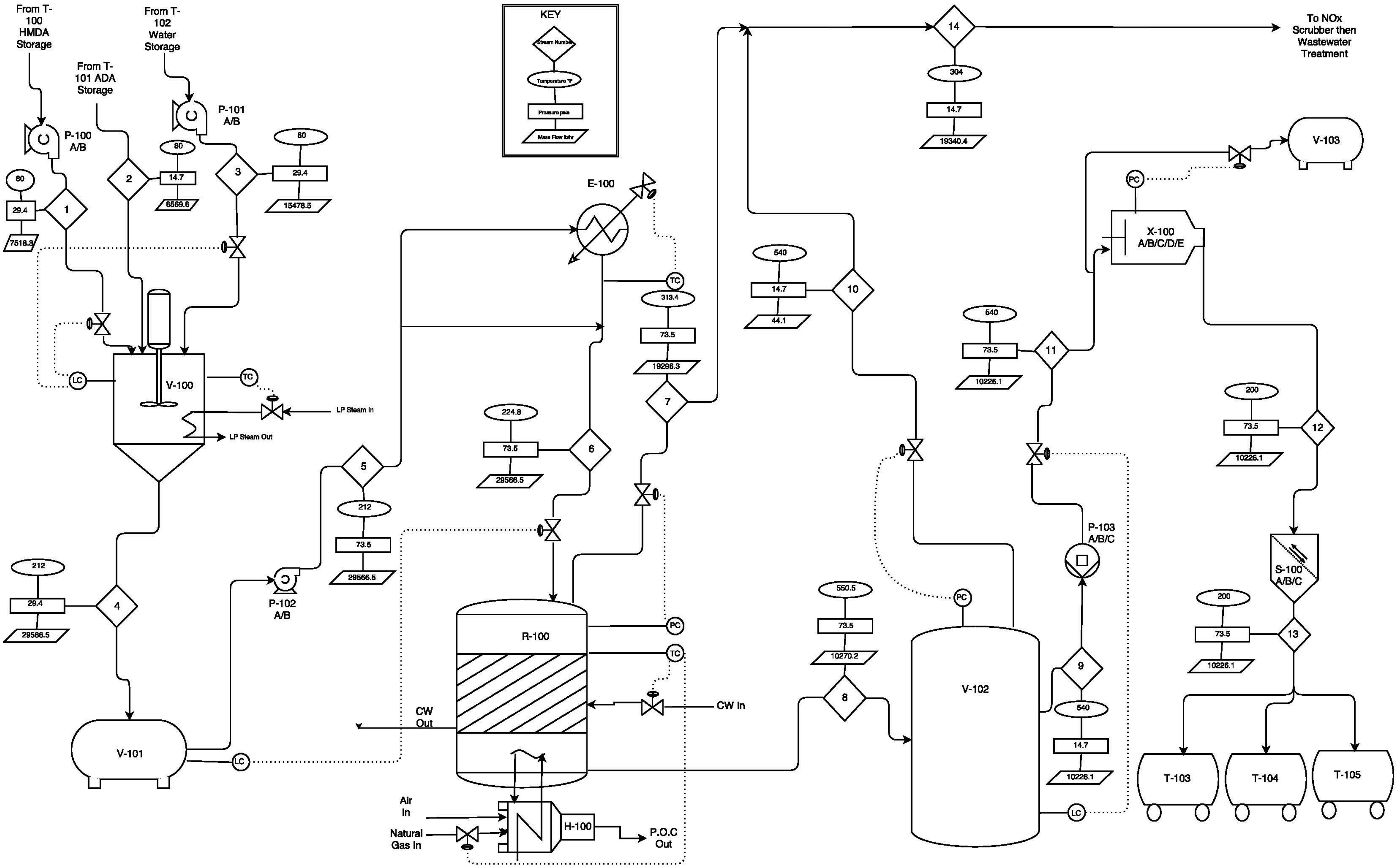
Figure 1. Batch Process Flow Diagram



Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Stream Description	HMDA Flow into V-200	ADA Flow into V-200	Water Flow into V-200	Nylon Salt Flow from V-200	Nylon Salt Flow from V-200	Nylon Salt flow into R-200	Flow into V-202	Flow into R-201	Vapor Flow from V-202	Vapor Flow from R-201	Flow into P-203 A/B	Flow into X-200	Flow into S-201	Flow to Nylon-6,6 Storage	Flow to N_2O Scrubber

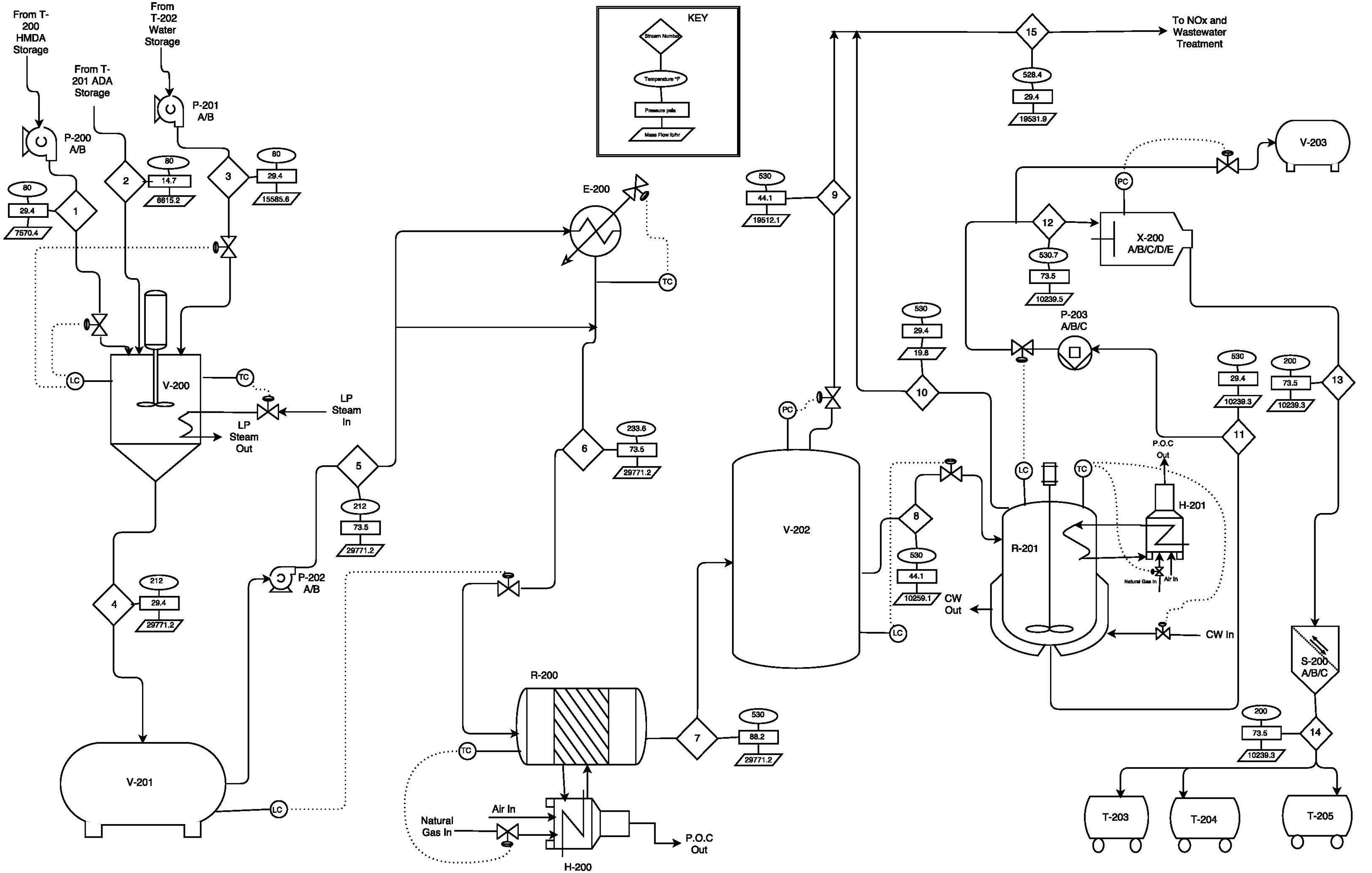
Figure 2. Continuous Process Flow Diagram

Once the process flow diagrams were drafted, the group developed a preliminary control system for the processes. The group evaluated every piece of equipment and processing step to ensure that the control design implemented would result in a safe and efficient method for the manufacturing of nylon-6,6. The process flow diagrams for each process and the control systems will be further explored in the Process Description section of this report. The batch process with controls is labeled as Figure 3 and the continuous process is labeled as Figure 4. They are shown in the following pages.



Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Stream Description	HMDA Flow into V-100	ADA Flow into V-100	Water Flow into V-100	Nylon Salt Flow from V-100	Nylon Salt Flow from V-101	Nylon Salt flow to R-100	Vapor Flow from R-100	Flow to V-102	Flow to P-103 A/B	Vapor Flow from V-102	Flow to X-100	Flow to S-101	Flow to Nylon-6,6 Storage	Flow to N_2O Scrubber

Figure 3. Batch Process Flow Diagram with Controls



Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Stream Description	HMDA Flow into V-200	ADA Flow into V-200	Water Flow into V-200	Nylon Salt Flow into V-201	Nylon Salt Flow from V-201	Nylon Salt flow into R-200	Flow into V-202	Flow into R-201	Vapor Flow from V-202	Vapor Flow From R-201	Flow into P-203 A/B	Flow into X-200	Flow into S-201	Flow to Nylon-6,6 Storage	Flow to N_2O Scrubber

Figure 4. Continuous Process Flow Diagram with Controls

Mass Balances

The group conducted a total mass balance, and it was consistent with mass conservation for both processes. The results are shown in Tables 1 and 2 below.

Table 1. Batch Process Mass Balance

Batch Design		
Species	**Inlet Process Mass Flow (lb / hr)**	**Outlet Process Mass Flow (lb / hr)**
ADA	6564	0
HMDA	5263	9
Water	17734	19338
Nylon-6,6	0	10214
N_2O	6	6
Total	29567	29567

Table 2. Continuous Process Mass Balance

Continuous Design		
Species	**Inlet Process Mass Flow (lb / hr)**	**Outlet Process Mass Flow (lb / hr)**
ADA	6609	2
HMDA	5299	78
Water	17857	19471
Nylon-6,6	0	10214
N_2O	6	6
Total	29771	29771

Mole Balances

Mole balances were also performed for the batch and the continuous process designs. The material balance was based on the following condensed reversible reaction[17].

$$ADA + HMDA \leftrightarrow Nylon\ 6{,}6 + 2H_2O$$

The carboxylic acid group in ADA reacts with one of the two amine groups in HMDA to form nylon-6,6 and two molar equivalents of water. For basic description in elementary rate laws, the forward and reverse reactions can be described by the equations below. The values for the constant and activation energy are taken from Process Analysis and Simulation Engineering[17].

$$r_{fwd} = 7[COOH][NH_2]e^{\frac{-2.5*10^6 \frac{J}{kmol}}{RT}} \tag{1}$$

$$r_{rev} = 0.014[H_2O]e^{\frac{-2.5*10^6\frac{J}{kmol}}{RT}} \tag{2}$$

The general mole balance outline is described below. The balances were generated following the method outlined in the Fogler *Chemical Reaction Engineering* textbook[22].

For the batch process, the component mole balances are:

$$\frac{dN_{ADA}}{dt} = \left(-r_{fwd} + \frac{1}{2}r_{rev}\right) * V \tag{3}$$

$$\frac{dN_{ADA}}{dt} = \left(-r_{fwd} + \frac{1}{2}r_{rev}\right) * V \tag{4}$$

$$\frac{dN_{Nylon}}{dt} = \left(r_{fwd} - \frac{1}{2}r_{rev}\right) * V \tag{5}$$

$$\frac{dN_{Water}}{dt} = \left(2r_{fwd} - r_{rev}\right) * V \tag{6}$$

Initial conditions for the process are 984.36 lbmol of water, 44.91 lbmol of ADA, and 45.29 lbmol of HMDA, these values were selected to achieve the necessary nylon-6,6 output. The volume of the batch reactor used was 46.7 cubic meters, and was calculated using the total cycle time and volumetric flows of process streams.

The reactor is assumed to be isothermal at 550 °F, the reaction is taking place in the liquid phase, and the reactants are in the batch reactor for two hours[5][17].

For the continuous process, the material balance around the PFR is described by the following equations.

$$\frac{dF_{ADA}}{dV} = \left(-r_{fwd} + \frac{1}{2}r_{rev}\right) \tag{7}$$

$$\frac{dF_{HMDA}}{dV} = \left(-r_{fwd} + \frac{1}{2}r_{rev}\right) \tag{8}$$

$$\frac{dF_{Nylon}}{dV} = \left(r_{fwd} - \frac{1}{2}r_{rev}\right) \tag{9}$$

$$\frac{dF_{Water}}{dV} = \left(2r_{fwd} - r_{rev}\right) \tag{10}$$

Initial conditions for the process are 991.2 lbmol per hour of water, 45.22 lbmol per hour of ADA, 45.6 lbmol per hour of HMDA. The final volume of the PFR used was optimized to be 35.6 cubic meters. Like the batch process, the reactor is assumed to be isothermal at 530 °F and the reaction is taking place primarily in the liquid phase[5][17].

The group also checked both Aspen simulations to ensure that the molar flows in and out of the process align with the material balance results. Assuming the forward reaction goes to near completion, the following tables describe the moles of each species at the beginning and end of each process from the simulation versus the approximate hand calculation. For the batch process, the values for the outlet process molar flow match the material balance calculations. The slight variation is due to the more complex polymerization reaction kinetics as well as the presence of nitrous oxide affecting the final conversion of the reaction[39].This is demonstrated in Table 3.

Table 3. Batch Process Mole Balances

Batch Design			
Species	**Inlet Process Molar Flow (lbmol / hr)**	**Outlet Process Molar Flow (lbmol / hr)**	**Outlet Material Balance Molar Flow (lbmol / hr)**
Adipic Acid	44.91	0.00	0.00
HMDA	45.29	0.72	0.38
Water	984.36	1073.36	1074.18
Nylon 6,6	0.00	45.13	44.91
N_2O	0.13	0.13	0.13
Total	1074.69	1119.34	1119.60

The same process was conducted on the continuous design, and the results can be seen below.

Table 4. Continuous Process Mole Balances

Continuous Design			
Species	**Inlet Process Molar Flow (lbmol / hr)**	**Outlet Process Molar Flow (lbmol / hr)**	**Outlet Material Balance Molar Flow (lbmol / hr)**
Adipic Acid	45.22	0.02	0.00
HMDA	45.60	0.68	0.38
Water	991.20	1080.39	1081.64
Nylon 6,6	0.00	45.15	45.22
N_2O	0.14	0.14	0.14
Total	1082.16	1126.38	1127.38

Stream Tables

When drafting the process flow diagrams that were shown in a previous subsection, stream labels were assigned throughout the diagram. The corresponding stream tables have been drafted and are shown in the next pages. The stream table for the batch process is labeled as Table 5 and the continuous process stream table is labeled as Table 6. It should be noted that all mass and mole balances are in agreement with the results displayed in the stream tables.

Table 5. Batch Process Stream Table

Batch Process														
Stream Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Stream Description	HMDA flow into V-100	ADA flow into V-100	Water flow V-100	Nylon Salt flow from V-100	Nylon Salt flow from V-101	Nylon Salt flow to R-100	Vapor flow from R-100	Flow to V-102	Flow to P-103 A/B	Vapor Flow from V-102	Flow to X-100	Flow to S-101	Flow to Nylon-6,6 Storage	Flow to N_2O Scrubber
Properties														
Temperature (°F)	80.0	80.0	80.0	212.0	212.0	224.8	313.4	550.5	540.0	540.0	540.0	200.0	200.0	304.0
Pressure (psia)	29.4	14.7	29.4	29.4	73.5	73.5	73.5	73.5	14.7	14.7	73.5	73.5	73.5	14.7
Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
Mass Flow (lb/hr)	7518.3	6569.6	15478.5	29566.5	29566.5	29566.5	19296.3	10270.2	10226.1	44.1	10226.1	10226.1	10226.1	19340.4
Component Mass Flow (lb/hr)														
HMDA	5262.80	0.00	0.00	5262.84	5262.84	5262.84	8.75	0.78	0.56	0.22	0.56	0.56	0.56	8.97
ADA	0.00	6563.67	0.00	6563.67	6563.67	6563.67	0.29	0.20	0.20	3.42E-03	0.20	0.20	0.20	3.23E-02
Water	2255.50	0.00	15478.50	17734.00	17734.00	17734.00	19281.60	55.28	11.41	43.87	11.41	11.41	11.41	19325.49
Nylon-6,6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	10213.93	10213.93	3.78E-77	10213.93	10213.93	10213.93	3.78E-77
Nitrous Oxide	0.00	5.91	0.00	5.91	5.91	5.91	5.92	0.00	0.00	0.00	0.00	0.00	0.00	5.91484
Mole Flow (lbmol/hr)	170.50	45.05	859.20	1074.72	1074.72	1074.72	1070.50	48.21	45.77	2.44	45.77	45.77	45.77	1072.94
Component Molar Flow (lbmol/hr)														
HMDA	45.29	0.00	0.00	45.29	45.29	45.29	0.71	6.74E-03	4.86E-03	1.88E-03	4.86E-03	4.86E-03	4.86E-03	7.71E-02
ADA	0.00	44.91	0.00	44.91	44.91	44.91	2.00E-04	1.37E-03	1.35E-03	2.34E-05	1.35E-03	1.35E-03	1.35E-03	2.21E-04
Water	125.20	0.00	859.20	984.36	984.36	984.36	1070.29	3.07	0.63	2.43	0.63	0.63	0.63	1072.73
Nylon-6,6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	45.13	45.13	1.67E-79	45.13	45.13	45.13	1.67E-79
Nitrous Oxide	0.00	0.13	0.00	0.13	0.13	0.13	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.13
Density (lb/ft^3)	52.90	91.47	60.18	56.73	56.73	56.24	0.16	53.41	53.64	2.48E-02	53.62	59.74	59.74	3.25E-02
Enthalpy (Btu/lb)	-2443.00	-2322.00	-6866.00	-4714.67	-4714.67	-4703.81	-5665.40	-488.75	-470.91	-5532.34	-470.28	-673.45	-673.45	-5665.24
Volumetric Flow (ft^3/hr)	142.12	71.82	257.34	501.34	521.20	525.75	117857.00	192.30	190.64	1774.58	190.70	171.18	171.18	595298.00

Table 6. Continuous Process Stream Table

Continuous Process															
Stream Number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
Stream Description	HMDA Flow into V-200	ADA Flow into V-200	Water Flow into V-200	Nylon Salt Flow into V-201	Nylon Salt flow from V-201	Nylon Salt Flow into R-200	Flow into V-202	Flow into R-201	Vapor Flow from V-202	Vapor Flow from R-201	Flow into P-203 A/B	Flow into X-200	Flow into S-201	Flow to Nylon-6,6 Storage	Flow to N_2O Scrubber
Properties															
Temperature (°F)	80.0	80.0	80.0	212.0	212.0	233.6	530.0	530.0	530.0	530.0	530.0	530.7	200.0	200.0	528.4
Pressure (psia)	29.4	14.7	29.4	29.4	73.5	73.5	88.2	44.1	44.1	29.4	29.4	73.5	73.5	73.5	29.4
Vapor Fraction	0.00	0.00	0.00	0.00	0.00	0.00	0.96	0.00	1.00	1.00	0.00	0.00	0.00	0.00	1.00
Mass Flow (lb/hr)	7570.4	6615.2	15585.6	29771.2	29771.2	29771.2	29771.2	10259.1	19512.1	19.8	10239.3	10239.3	10239.3	10239.3	19531.9
Component Mass Flow (lb/hr)															
HMDA	5299.30	0.00	0.00	5299.27	5299.27	5299.27	79.45	1.51	77.95	4.89E-03	6.16E-02	6.16E-02	6.16E-02	6.16E-02	77.95
ADA	0.00	6609.21	0.00	6609.21	6609.21	6609.21	3.48	1.10	2.38	1.91E-03	5.80E-01	5.80E-01	5.80E-01	5.80E-01	2.38
Water	2271.13	0.00	15585.64	17856.77	17856.77	17856.77	19463.58	37.75	19425.83	19.77	24.77	24.77	24.77	24.77	19445.60
Nylon-6,6	0.00	0.00	0.00	0.00	0.00	0.00	10218.73	10218.73	1.47E-75	1.81E-78	10213.9	10213.9	10213.9	10213.9	1.47E-75
Nitrous Oxide	0.00	5.95	0.00	5.95	5.95	5.95	5.95	2.51E-03	5.95	1.97E-03	5.37E-04	5.37E-04	5.37E-04	5.37E-04	5.95
Mole Flow (lbmol/hr)	171.70	45.36	865.20	1082.16	1082.16	1082.16	1126.39	47.27	1079.12	1.10	46.51	46.51	46.51	46.51	1080.22
Component Molar Flow (lbmol/hr)															
HMDA	45.60	0.00	0.00	45.60	45.60	45.60	0.68	1.30E-02	0.67	4.21E-05	5.30E-04	5.30E-04	5.30E-04	5.30E-04	0.67
ADA	0.00	45.22	0.00	45.22	45.22	45.22	2.38E-02	7.55E-03	1.63E-02	1.31E-05	3.97E-03	3.97E-03	3.97E-03	3.97E-03	1.63E-02
Water	126.07	0.00	865.20	991.20	991.20	991.20	1080.39	2.10	1078.30	1.10	1.38	1.38	1.38	1.38	1079.40
Nylon-6,6	0.00	0.00	0.00	0.00	0.00	0.00	45.15	45.15	6.51E-78	7.99E-81	45.13	45.13	45.13	45.13	6.52E-78
Nitrous Oxide	0.000	0.135	0.000	0.135	0.135	0.135	0.135	5.71E-05	0.135	4.49E-05	1.22E-05	1.22E-05	1.2203E-05	1.2203E-05	0.135
Density (lb/ft^3)	52.90	91.47	60.18	58.43	56.73	55.90	0.23	53.81	7.56E-02	5.01E-02	53.84	53.82	59.79	59.79	5.04E-02
Enthalpy (Btu/lb)	-2443.00	-2332.00	-6866.00	-4719.00	-4714.67	-4696.26	-3807.71	-502.53	-5541.69	-5562.65	-490.70	-490.23	-687.26	-687.26	-5541.71
Volumetric Flow (ft^3/hr)	157.56	72.31	250.08	504.84	524.80	532.62	1.28E+05	190.64	2.58E+05	394.68	190.20	190.24	171.26	171.26	3.88E+05

Process Description

The process was modeled using Aspen Plus Polymers simulation software. The overall reaction is as follows:

Overall Reaction	
$HDMA + ADA \leftrightarrow 2\,WATER + NYLON\ 6{,}6$	(1)

The reaction kinetics follow a step-growth polymerization reaction[17]. The step-growth reactions are as follows:

Condensation Reactions	
$HDMA + ADA \leftrightarrow WATER + HMDA - E + ADA - E$	(2)
$HDMA + ADA - E \leftrightarrow WATER + HMDA - E + ADA - R$	(3)
$HDMA - E + ADA \leftrightarrow WATER + HMDA - R + ADA - E$	(4)
$HDMA - E + ADA - E \leftrightarrow WATER + HMDA - R + ADA - R$	(5)
Polymerization Reactions	
$HDMA + ADA - E + HDMA - R \leftrightarrow 2HDMA - E + ADA - E$	(6)
$HDMA + ADA - R + HDMA - R \leftrightarrow 2HDMA - E + ADA - R$	(7)

The rates utilized are listed in the material balance section above[17]. The step-growth reactions shown above were developed by the POLYNRTL database within Aspen Plus. In order to accurately model the process within the software the group located documentation that would outline the proper techniques to model both the batch and continuous processes. This documentation allowed the group to follow a process that was logical and would accurately predict nylon-6,6 yield[17].

For the batch reaction the group elected to follow the process described in several industrial applications and the outline provided in the Aspen simulation walkthrough[17][27]. The batch process that was modeled in the software can be seen in the image below.

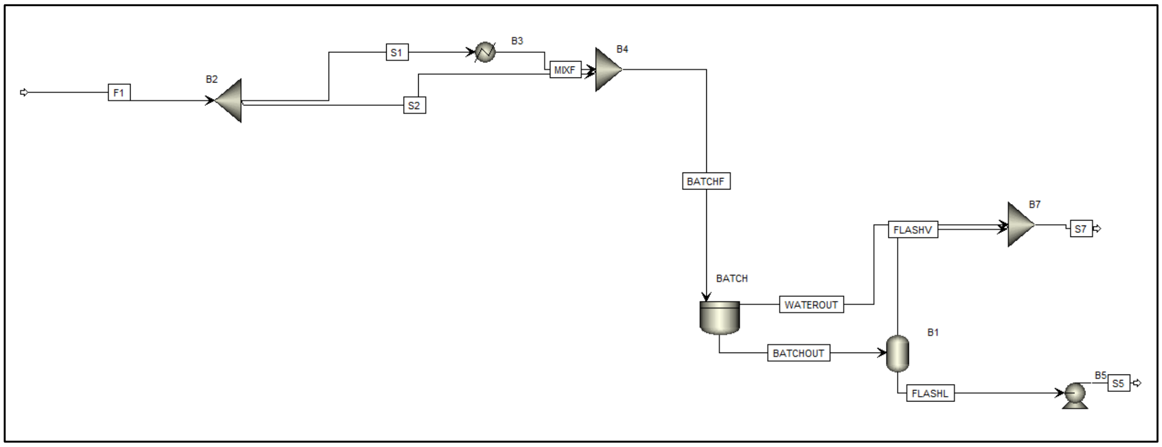


Figure 5. Batch Process Aspen Simulation

In order to model the continuous process the group utilized a plug flow reactor in series with a CSTR[17]. The documentation utilized also gave optimum process temperatures and pressures that they discovered. However, through rigorous simulation and optimization the group found a scenario that resulted in a higher nylon-6,6 yield without introducing unnecessary risks with extreme temperatures or pressures. A summary of the optimum process conditions can be viewed in Table 8. The continuous simulation utilized can be seen in the figure below. It should be noted that there are some upstream and downstream processes not shown in this simulation figure.

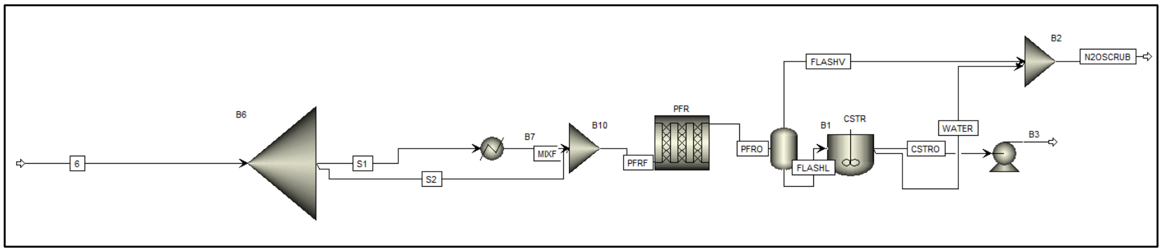


Figure 6. Continuous Process Aspen Simulation

Block Flow Diagrams

The processes were evaluated on a ground level before the preliminary design process began. The overall process was put into a block flow diagram that shows the nylon-6,6 production process via the simplified processing steps. The block flow diagram for the batch process is labeled as Figure 7 and the block flow diagram for the continuous process is labeled as Figure 8.

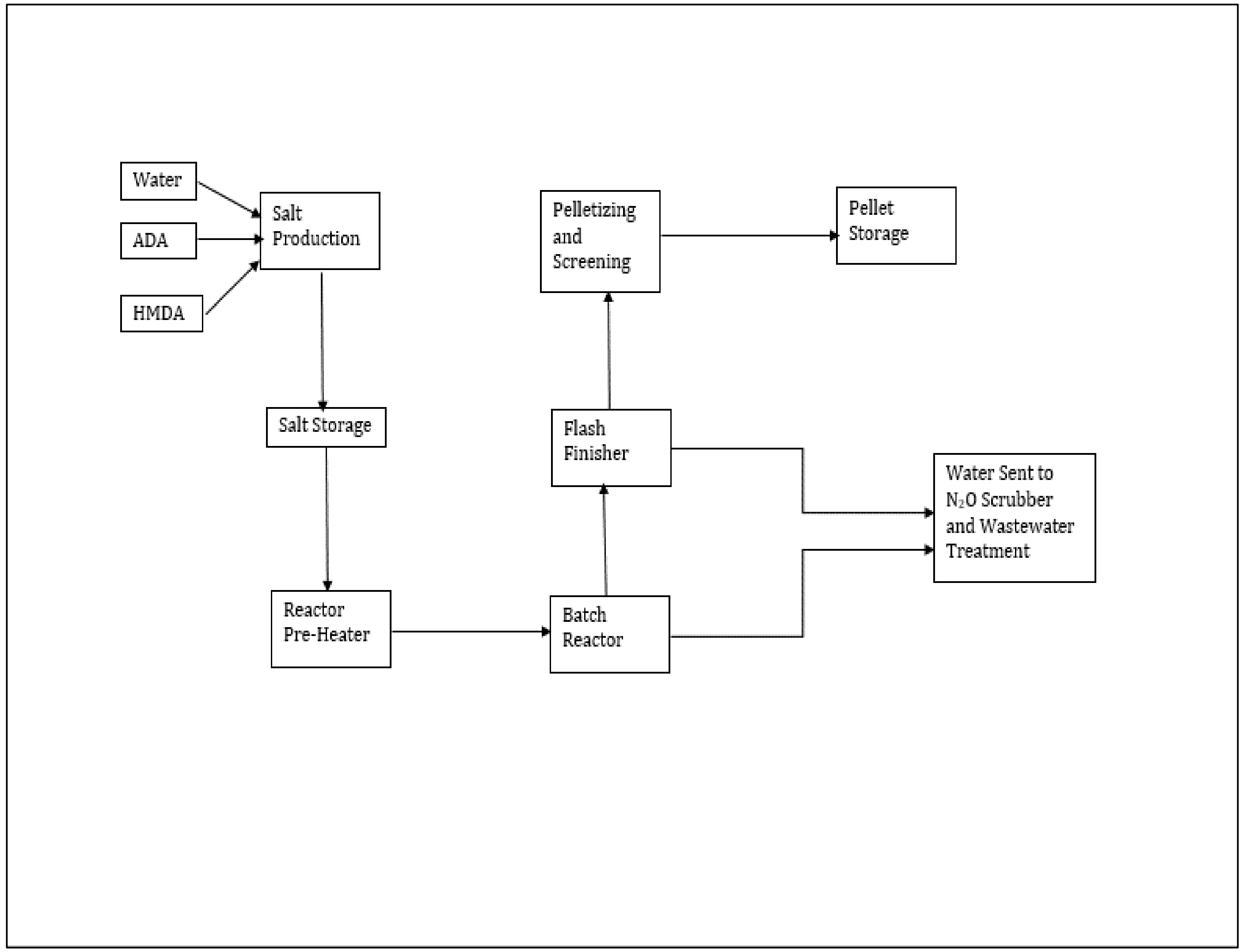


Figure 7. Batch Process Block Flow Diagram

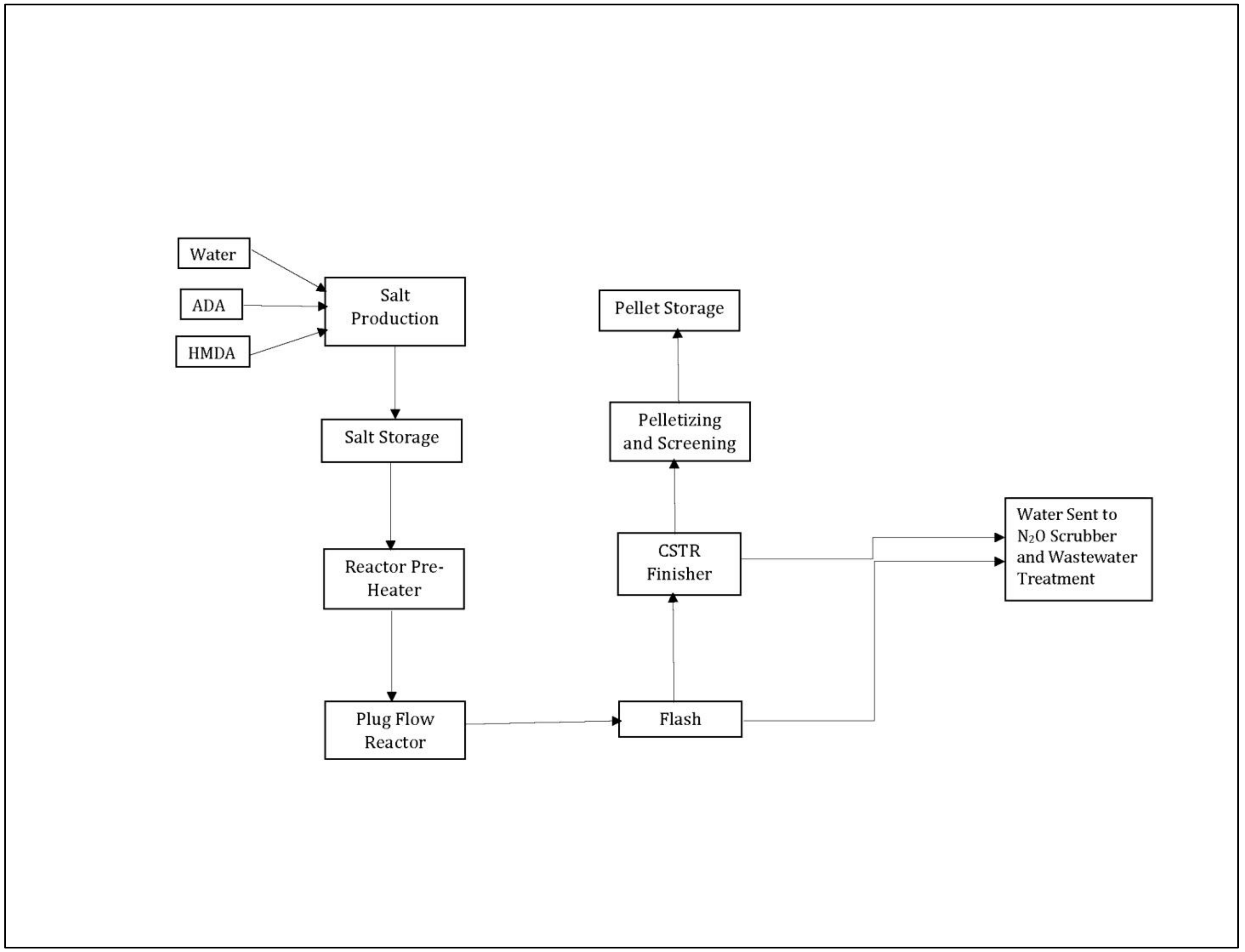


Figure 8. Continuous Process Block Flow Diagram

Batch

The batch process begins with the transport of the raw materials, stream 1 (HMDA), stream 2 (ADA), and stream 3 (deionized water), to the process, and they are combined in a heated mixer, V-100, to begin the production of nylon-6,6 salt solution. V-100 is heated by a flow of low pressure steam, where the flow is controlled by a control valve according to the temperature measured in the mixer. The level in V-100 is also monitored via a control system and is adjusted by changing the flows of the water and HMDA into the mixer. Following the salt solution production, the mixture is stored as an intermediate in V-101 before being transported to the batch reactor, R-100. The salt storage vessel level is controlled via a level controller and control valve attached to stream 6.

After the salt solution leaves the storage vessel, the stream is split and a portion of the salt solution is heated in E-100 so that the water will immediately separate from the nylon-6,6 product once the solution is introduced to the reactor[50]. The separation of water is key to the reaction because this promotes the condensation of the nylon-6,6 polymer. Heater E-100's temperature differential is controlled by a temperature controller on stream 6 that operates a control valve on the low pressure steam line. When exploring the effects of pre-heating the feed to R-100, the group optimized the amount of salt solution that was fed through the heater, as well as the temperature change the heater induced to the feed to the reactor (Table 7). Once the salt solution is introduced into the reactor, the polycondensation reaction begins. R-100 is maintained at a constant temperature of 550°F with a steady cycle of utilities, including Paratherm HT and cooling water. The Paratherm HT is heated via furnace H-100, and is connected to R-100 with coils while the cooling water system is within the jacket of the reactor. The reaction is exothermic so it is imperative to maintain the reactor at a constant temperature[5]. The temperature of R-100 was another variable that was optimized through the Aspen Plus software (Table 7). Knowing that the temperature of the reactor had to above the melting temperature of nylon-6,6 to prevent the formation of the solid polymer within the reactor, the group optimized the temperature to be 550°F so that the most nylon-6,6 was produced. The water that is separated in R-100 is vented from the reactor and is then transported the N_2O scrubber via stream 7. As this is a vapor stream, the flow of this stream is changed with a control valve and pressure controller to maintain the pressure of R-100.

The batch reactor has a reactor feed time that was optimized to 2 hours and once the 2 hours is complete, the nylon-6,6 product is transported to a flash tank, labeled V-102. Within the flash tank most of the remaining water that is in the nylon-6,6 product is flashed and transported to the N_2O scrubber through stream 10. Stream 7 and 10 are combined to form stream 14. The pressure within the flash tank is controlled in the same way that the pressure in R-100 is controlled. The level is also controlled within V-102 via a control valve on stream 11, the discharge side of the positive displacement pump. P-103 was put into the process so that the molten nylon could be transported to the final steps of the process. A positive displacement was chosen over a more common centrifugal pump because the molten nylon is a viscous material that a centrifugal pump would not be able to process.

At this point in the process the nylon product has been fully manufactured and the processing steps remaining are the finishing steps. The first in this finishing process is the extruder, X-100. The extruder forces the molten nylon through a die and decreases the temperature, which will make the nylon solidify. As the nylon leaves the extruder, the nylon is cut into pellets. Within this process, if the die was to become plugged the pressure within the extruder could increase to dangerous levels. A pressure controller was implemented on stream 11 that, if employed, would divert the molten nylon to an emergency storage vessel, V-103. Once the cut pellets leave the extruder, they enter in to a vibrating screen, S-101, that will separate the pellets by size to ensure that the product that will be delivered to consumers at the required size specifications. Once the finished pellets leave the screen, they are transported to the final product storage, labeled as T-103 through T-105 on the PFD for the batch process.

Continuous

The continuous process that was designed contains many of the same processing steps as the batch process. The two process flow diagrams are similar, with the main differences being some flow rates and slightly different temperatures, from the start of the process until the input to the reactors. This corresponds to streams 1 through 6 on both PFDs.

Starting with the salt solution entering the PFR, R-200, the salt precipitation reaction takes place at a temperature of 530°F, which is maintained through a flow of Paratherm HT that is heated via H-200. The control system adjusts the flow of natural gas into the furnace. The precipitate product is moved to a flash tank, V-202, where water is removed to prepare the product for the polycondensation reaction that will take place in R-201. Much like in the batch process, the pressure in V-202 is controlled via the vapor flow rate of stream 9 out of the flash tank. The level in V-202 is also controlled by changing the outlet liquid flow from V-202.

The precipitation product now enters a CSTR, R-201 that also removes water via stream 10 and condenses the precipitate product into molten nylon. Within R-201 the level and temperature is controlled. The level is controlled by changing the flow rate of the discharge on P-203, similar to the control mechanism for the level on V-102 in the batch process. The water removed in V-202 and R-201 is transported to the N_2O scrubber for waste treatment by stream 15.

After R-201, the processing steps are the synonymous to the batch process that was described in the previous subsection. The corresponding streams are streams 11 through 14 for the continuous process and streams 9 through 13 for the batch process.

The continuous process was selected by the group for a multitude of reasons including: economics, personnel exposure, and ease of operation. Through the description of the continuous option it is concluded that this is a streamlined option. Additionally, with the continuous process the group can eliminate the need for frequent reactor cleaning, which leads to decreased personnel exposure. Furthermore, the continuous model is utilized in several industrial application and has been for more than six decades[10][27].

Optimization

As referenced earlier, optimization within the Aspen Plus software was completed to ensure that operating conditions within the process would result in the greatest production of nylon-6,6. For the batch process, optimization was completed for the feed temperature, the percent of feed being heated in E-100, the temperature for R-100 and the pressure for R-100. To adjust the feed temperature, the temperature gradient of E-100 was adjusted within the Aspen Plus simulation. For the continuous process, optimization was completed for the temperature of R-200, the pressure of R-200, the volume of R-200, the temperature of R-201, the percent of feed being heated in E-200, and the pressure of R-201. There were some overlap in optimum conditions between the batch and continuous processes, such as the heater temperature gradient. It is important to note that the PFR volume was optimized assuming a constant L/D ratio during this stage of optimization. Some of the optimum operating conditions were changed during the economic optimization process, and this is further discussed in the Economic Analysis section of this report. The final values chosen for the various areas of the processes are shown in Tables 7 and 8. Tables A2 through A11, detailing the entire optimization process, are shown in the Appendix of this report.

Table 7. Optimization Results: Batch Process

Feed Temperature to R-100	224.8 °F
R-100 Temperature	550 °F
R-100 Pressure	5 atm (73.5psia)
Percent of Feed Being Heated	29.4%

Table 8. Optimization Results: Continuous Process

R-200 Temperature	530 °F
R-200 Pressure	6 atm (88.2psia)
R-200 Volume (based on L/D=25)	4241.2 ft^3 (Length=150ft; Diameter=6ft)
Percent of Feed Being Heated	29.4%

R-201 Temperature	530 °F
R-201 Pressure	2 atm (29.4psia)

Energy Balance and Utility Requirements

Batch Reactor Energy Balance

The energy balance for the batch reactor is shown first. As there is no flow in or out of the reactor during the reaction, all flow terms are eliminated from the energy balance. The heat produced by the series of reactions subtracted from the heat added will be proportional to the change in temperature in the reactor[22].

$$\rho C_p V_{batch} \frac{dT}{dt} = \dot{Q} - \sum \Delta H_{rxn,i} r_i \, V_{batch} \tag{11}$$

The group is modeling the batch reactor as an isothermal reactor at 550 °F, so the equation reduces to the following.

$$\dot{Q} = \sum \Delta H_{rxn,i} r_i \, V_{batch} \tag{12}$$

So, the heat added to the batch reactor is equal to the sum of the heats of reaction multiplied by the rates of those reactions.

PFR Energy Balance

The energy balance for the PFR in the continuous design follows similar logic. The flow through the reactor is included in the energy balance as well as the pressure drop down the reactor. The initial energy balance looks like the following[22].

$$F \rho C_p V_{PFR} \frac{dT}{dV} + F \frac{dP}{dV} = \dot{Q} - \sum \Delta H_{rxn,i} r_i \, V_{PFR} \tag{13}$$

For isothermal operation, the PFR energy balance adds a pressure term to the batch energy balance. The PFR energy balance is shown below.

$$\dot{Q} = \sum \Delta H_{rxn,i} r_i V_{PFR} + F V_{PFR} \frac{dP}{dV} \tag{14}$$

CSTR Energy Balance

The energy balance for the CSTR, also included in the continuous process is similar to the other two, but it adds a flow term to the batch energy balance. So, rather than the initial equation being synonymous to Equation (13), the energy balance becomes the following equation[22].

$$\rho C_p V_{CSTR} \frac{dT}{dt} = \dot{Q} - \sum \Delta H_{rxn,i} r_i V_{CSTR} + \sum F_{0,i}(H_{in,i} - H_{out,i}) \tag{15}$$

With the isothermal operation assumption used in the project, the above equation reduces to the isothermal CSTR energy balance.

$$\dot{Q} = \sum \Delta H_{rxn,i} r_i V_{CSTR} + \sum F_{0,i}(H_{in,i} - H_{out,i}) \tag{16}$$

The amount of heat required for the CSTR is given by the parameter $\dot{Q}$.

Overall Energy Balance

Each energy balance was performed in Aspen Plus. The heat added to each reactor in the simulations was calculated using the heat of reaction, flow characteristics, and pressure in the specific reactor. This results in the following energy balance:

$$0 = \frac{dE}{dt} = E_{in} - E_{out} + E_{gen} \tag{17}$$

The group performed manual calculations to validate that the overall energy balance equals zero for the processes simulated in Aspen Plus. The group summed the inlet energy and outlet energy for each case, to ensure energy closure. The energy generated by the reaction was factored into the Aspen Plus calculation of each reactors duty. The batch process has an energy accumulation of 0.28% of the energy supplied. The continuous process has an energy accumulation of approximately 0% of the energy supplied. The accumulation found in the batch process was attributed to rounding in the group's calculations.

Table 9. Overall Energy Balance Results

	Batch (BTU/h)	Continuous (BTU/h)
Energy In	113264486	114706000
Energy Out	113264501	114383600
Energy Accumulated	-15	322400
Percentage of Inlet	0%	0.28%

Utility Requirements

Initially, the reactors must be heated to get the reactor contents to the optimum reaction temperature. The optimum reaction temperature is 550 °F for the batch process (Table 7) and 530 °F for the continuous process (Table 8). In each process, hot oil flows through a coil within the reactors to heat the contents to the appropriate temperature. This hot oil is heated with a furnace and is recycled between the reactor and the furnace. Paratherm HT was selected as the oil as it is rated for temperatures from 52 °F to 650 °F and designed for looped furnace heating applications[46].

Once the reaction is initiated heat is given off, as the reaction forming nylon-6,6 is exothermic[5]. In order to prevent a runaway reaction, cooling water is also required. When the reactor reaches a temperature 5 degrees above the desired temperature, a controls system will shut off the hot oil feed and begin the flow of cooling water through the reactor jacket. The cooling water properties supply temperature of 104 °F was taken from heuristics[62]. A return temperature of 113 °F was assumed.

For the batch simulation, the reactor is initially heated and then cooled for the remainder of the reaction time. The heat exchangers associated with the hot oil and cooling water for the batch reactor were sized and costed.

For the continuous simulation, neither the PFR nor CSTR required cooling. As a result, the cooling water heat exchanger included in the PFR and CSTR could not be costed. However, a cooling water system is still in place for both reactors within the design. Further investigation should be done in detailed design to understand the duty profile within the PFR and CSTR and the costs associated with the cooling required.

Additional utilities include low pressure steam, electricity and natural gas. The low-pressure steam is used to heat the contents of the nylon salt mixer and the stream in the pre-feed heater. The properties for the low-pressure steam are as shown in

Table 10 below[62]. An approach temperature of 20 °F was assumed for all heat exchangers using low pressure steam.

Table 10. Low Pressure Stream Specifications

Low Pressure Steam Supply Temperature	320 °F
Low Pressure Steam Supply Pressure	5 barg
Low Pressure Steam Approach Temperature	20 °F

The electricity is used to power all the pumps, mixers, and extruders within the process. The natural gas is used in the furnace and the N_2O scrubber.

Equipment List and Unit Descriptions

Batch

Table 11. Batch Process Equipment List

Equipment ID	Equipment Name	Quantity	Equipment Description
R-100	Batch Reactor	1	Stainless steel reactor that carries out the step-growth polymerization reaction to form nylon-6,6.
H-100	Fired Heater	1	Stainless steel furnace that utilizes Paratherm HT to heat reactor to specified temperature to induce step-growth reaction.
P-100	Reciprocating Pump	2	Titanium pump that transports HMDA from storage to heated mixing tank V-100.
P-101	Centrifugal Pump	2	Stainless steel pump that transports deionized water from storage to heated mixing tank V-100.
P-102	Centrifugal Pump	2	Stainless steel pump that increases pressure from salt storage to transfer to R-100.
P-103	Positive Displacement Pump	3	Stainless steel pump that pumps molten nylon-6,6 product to densification and extrusion process.

M-100	Tank Mixer	2	Stainless steel mixer that ensures contents of salt tank are well mixed prior to feeding into R-100.
E-100	Pre-Feed Heat Exchanger	1	Shell and tube heat exchanger that pre-heats feed to reactor to ensure proper vapor-liquid interaction within R-100.
V-100	Salt Solution Mixer	1	Stainless steel vessel with mixer and steam heater that mixes and heats salt solution to 212°F prior to introduction into the R-100.
V-101	Salt Solution Storage	1	Stainless steel vessel that stores well mixed salt solution prior to introduction into reactor.
V-102	Flash Tank	1	Stainless steel flash tank that removes water from the process to meet final product purity specifications.
V-103	Emergency Nylon Storage	1	Stainless steel vessel that serves as an emergency storage tank to hold molten nylon in case of extruder shutdown.
T-100	Fixed Roof Tank	1	API Fixed roof tank that stores 30 days of the HMDA aqueous solution.
T-101	Fixed Roof Tank	1	API Fixed roof tank that stores 30 days of the ADA solid powder.
T-102	Fixed Roof Tank	1	API Fixed roof tank that stores 30 days of deionized water.
T-103	Fixed Roof Tank	1	API Fixed roof tank that stores 30 days of nylon-6,6 pellets.
S-100	Vibrating Screen	3	Vibrating sifting screen that ensures that formed nylon-6,6 pellets meet

			product size specifications.
Cv-100	Belt Conveyor	1	Enclosed belt conveyor that transports solid ADA from storage to heated mixing tank.
Ch-100	Auto-Dumping Chute	1	Automated chute that introduces ADA transported from the conveyor to V-100.
X-100	Double-Screw Extruder	5	Double screw extrusion and pelletizing machine that takes molten nylon-6,6 and transforms it to solid pellets to be sent to screens.
Sc-100	Nitrous Oxide Scrubber	1	Low NOx burner and flue gas recycle scrubber that removes nitrous oxide from waste water streams to meet environmental specifications.

Continuous

Table 12. Continuous Process Equipment List

Equipment ID	Equipment Name	Quantity	Equipment Description
R-200	Plug Flow Reactor	1	Stainless steel reactor that carries out the precipitation portion of the reaction to form nylon-6,6.
R-201	CSTR Reactor	1	Stainless steel reactor that carries out the polycondensation reaction to form nylon-6,6.
H-200	Fired Heater	1	Stainless steel furnace that utilizes Paratherm HT to heat the PFR to specified temperature to induce step-growth reaction.

H-200	Fired Heater	1	Stainless steel furnace that utilizes Paratherm HT to heat the CSTR to specified temperature to induce step-growth reaction.
P-200	Reciprocating Pump	2	Titanium pump that transports HMDA from storage to heated mixing tank V-200.
P-201	Centrifugal Pump	2	Stainless steel pump that transports deionized water from storage to heated mixing tank V-200.
P-202	Centrifugal Pump	2	Stainless steel pump that increases pressure from salt storage to transfer to R-200.
P-203	Positive Displacement Pump	3	Stainless steel pump that pumps molten nylon-6,6 product to densification and extrusion process.
M-200	Tank Mixer	2	Stainless steel mixer that ensures contents of salt tank are well mixed prior to feeding into R-200.
E-200	Pre-Feed Heat Exchanger	1	Shell and tube heat exchanger that pre-heats feed to reactor to ensure vapor-liquid interaction within R-200.
V-200	Salt Solution Mixer	1	Stainless steel vessel with mixer and steam heater that mixes and heats salt solution to 212°F prior to introduction into the R-200.
V-201	Salt Solution Storage	1	Stainless steel vessel that stores well mixed salt solution prior to introduction into R-200.
V-202	Flash Tank	1	Stainless steel flash tank that removes water from the process to meet final product purity specifications.

V-203	Emergency Nylon Storage	1	Stainless steel vessel that serves as an emergency storage tank to hold molten nylon in case of extruder shutdown.
T-200	Fixed Roof Tank	1	API Fixed roof tank that stores 30 days of the HMDA aqueous solution.
T-201	Fixed Roof Tank	1	API Fixed roof tank that stores 30 days of the ADA solid powder.
T-202	Fixed Roof Tank	1	API Fixed roof tank that stores 30 days of deionized water.
T-203	Fixed Roof Tank	1	API Fixed roof tank that stores 30 days of nylon-6,6 pellets.
S-200	Vibrating Screen	3	Vibrating sifting screen that ensures that formed nylon-6,6 pellets meet product size specifications.
Cv-200	Belt Conveyor	1	Enclosed belt conveyor that transports solid ADA from storage to heated mixing tank.
Ch-200	Auto-Dumping Chute	1	Automated chute that introduces ADA transported from the conveyor to the heated mixing tank.
X-200	Double-Screw Extruder	5	Double screw extrusion and pelletizing machine that takes molten nylon-6,6 and transforms it to solid pellets to be sent to screens.
Sc-200	Nitrous Oxide Scrubber	1	Low NOx burner and flue gas recycle scrubber that removes nitrous oxide from waste water streams to meet environmental specifications.

Equipment Specification Sheets

Batch Process

Reactor

Identification:	Item	Batch Reactor	**Date:**	3/9/2017
	Item No.	R-100	**By:**	4287
	No. Required	1		

Function: Carry out the step-growth polymerization reaction to form nylon-6,6

Operation: Standard

Materials Handled:	Feed (Liquid)	Liquid Prod.	Vapor Prod.
Quantity (lb/hr)	29566.5	10270.2	19296.3
Component Flow:			
Water	17734	55.3	19281.6
Nylon-6,6	0	10213.9	0
HMDA	5262.8	0.8	8.8
Adipic Acid	6563.7	0.2	0.3
N2O	5.9	0	5.9
Pressure:	5 atm	5 atm	5 atm
Temperature:	224.6°F	550°F	313.4°F

Design Data:				
	Volume:	1650 ft^3	Pressure:	108.8 psig
	Length:	28.8 ft	Heat Duty:	2.44e+7 Btu/hr
	Diameter:	8.9 ft	Vapor Phase:	0.654
	M.O.C:	S.S	Liquid Phase:	0.346
	Residence Time:	2 hr	Temperature:	1700°F
	Cycle Time:	3 hr	Utility Type:	Paratherm HT
	Reaction:	Step-Growth		

Furnace

Identification:	Item	Fired Heater	**Date:**	3/9/2017
	Item No.	H-100	**By:**	4287
	No. Required	1		

Function: Heat reactor to specified temperature to induce step-growth reaction

Operation: Standard

Materials Handled:

Quantity (kg/hr)	638553.5
Component Flow:	
Paratherm HT	615095
Air	22169.6
Natural Gas	1288.9
Pressure:	5 atm
Temperature:	600°F

Design Data:	Heat Duty:	64382 MJ/hr	U_o:	10 Btu/hr°Fft^2
	Efficiency:	40%	Desired Temp:	550°F
	M.O.C.:	S.S	Utility Temp:	600°F
	Coil Area:	15940 ft^2		

Pump

Identification:	Item	Recip.	**Date:**	3/9/2017
	Item No.	P-100	**By:**	4287
	No. Required	2		

Function: Pump HMDA from storage to heated mixing tank V-100

Operation: Standard

Materials Handled:	Suction	Discharge
Quantity (lb/hr)	7518.3	7518.3
Component Flow:		
Water	2255.5	2255.5
Nylon-6,6	0	0
HMDA	5262.8	5262.8
Adipic Acid	0	0
N2O	0	0
Pressure:	1 atm	2 atm
Temperature:	80°F	82°F

Design Data:	Shaft Power:	0.151 kW	Pressure:	64.7 psig
	Pressure Ratio:	2	Temperature:	1100°F
	Delta P:	1 atm	Process Material:	HMDA/Water
	M.O.C:	Titanium		

Pump

Identification:	Item	Centrifugal	**Date:**	3/9/2017
	Item No.	P-101	**By:**	4287
	No. Required	2		

Function: Pump deionized water from storage to heated mixing tank

Operation: Standard

Materials Handled:	Suction	Discharge
Quantity (lb/hr)	15478.5	15478.5
Component Flow:		
Water	15478.5	15478.5
Nylon-6,6	0	0
HMDA	0	0
Adipic Acid	0	0
N2O	0	0
Pressure:	1 atm	2 atm
Temperature:	80°F	82°F

Design Data:				
	Shaft Power:	0.2732 kW	Pressure:	64.7 psig
	Pressure Ratio:	2	Temperature:	1400°F
	Delta P:	1 atm	Process Material:	Water
	M.O.C:	C.S.		

Pump

Identification:	Item	Centrifugal	**Date:**	3/9/2017
	Item No.	P-102	**By:**	4287
	No. Required	2		

Function: Increase pressure from salt storage to transfer to reactor

Operation: Standard

Materials Handled:	Suction	Discharge
Quantity (lb/hr)	29566.5	29566.5
Component Flow:		
Water	17734	17734
Nylon-6,6	0	0
HMDA	5262.8	5262.8
Adipic Acid	6563.7	6563.7
N2O	5.9	5.9
Pressure:	2 atm	5 atm
Temperature:	210°F	212°F

Design Data:				
	Shaft Power:	1.651 kW	Pressure:	108.8 psig
	Pressure Ratio:	2.5	Temperature:	1700°F
	Delta P:	3 atm	Process Material:	Salt Mix
	M.O.C:	S.S.		

Pump

Identification:	Item	Pos. Displace	**Date:**	3/9/2017
	Item No.	P-103	**By:**	4287
	No. Required	3		

Function: Pump molten nylon-6,6 product to densification and extrusion process

Operation: Standard

Materials Handled:	Suction	Discharge
Quantity (lb/hr)	10226.1	10226.1
Component Flow:		
Water	11.4	11.4
Nylon-6,6	10213.9	10213.9
HMDA	0.6	0.6
Adipic Acid	0.2	0.2
N2O	0	0
Pressure:	2 atm	5 atm
Temperature:	540°F	540°F

Design Data:	Shaft Power:	0.1147 kW	Pressure:	108.8 psig
	Pressure Ratio:	2.5	Temperature:	1700°F
	Delta P:	3 atm	Process Material:	Nylon
	M.O.C:	S.S.		

Mixer

Identification:	Item	Tank Mixer		**Date:**	3/9/2017
	Item No.	M-100		**By:**	4287
	No. Required	2			

Function: Ensure contents of salt tank are well mixed prior to feeding into reactor

Operation: Standard

Materials Handled:	
Quantity (lb/hr)	29566.5
Component Flow:	
Water	17734
Nylon-6,6	0
HMDA	5262.8
Adipic Acid	6563.7
N2O	5.9
Pressure:	2 atm
Temperature:	212°F

Design Data:	Shaft Power:	1.076 kW	Pressure:	2 atm
	M.O.C:	S.S	Temperature:	1700°F
	Process Material:	Salt Mix		

Heat Exchanger

Identification:	Item	S/T Fixed		**Date:**	3/9/2017
	Item No.	E-100		**By:**	4287
	No. Required	1			

Function: Pre-heat feed to reactor to ensure vapor-liquid interaction within reactor

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	8692.6	8692.6
Component Flow:		
Water	5213.8	5213.8
Nylon-6,6	0	0
HMDA	1547.3	1547.3
Adipic Acid	1929.8	1929.8
N2O	1.7	1.7
Vapor Frac.:	0	0
Pressure:	5 atm	5 atm
Temperature:	212°F	255°F

Design Data:				
	Heat Duty:	3.3e+5 Btu/hr	Pressure:	108.8 psig
	FEMA Type:	AES	Temperature:	1400 F
	M.O.C.:	S.S/C.S.	Utility Flow:	340 lbm/hr
	Delta P:	0	Utility Type:	LPS
	Utility Temp:	489.2°F	Utility Presure:	5 barg
	Approach Temp.:	20°F	Phase Change:	Shell Side
	Heat Transfer Area:	3 m^2	U_o:	40 Btu/hr°Fft^2
	Process Flow:	Salt Mix	Delta T:	35°F

Vessels

Identification:	Item	Salt Mixer	**Date:**	3/9/2017
	Item No.	V-100	**By:**	4287
	No. Required	1		

Function: Mix and Heat salt solution to 212°F prior to introduction into the reactor

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	29566.5	29566.5
Component Flow:		
Water	17734	17734
Nylon-6,6	0	0
HMDA	5262.8	5262.8
Adipic Acid	6563.7	6563.7
N2O	5.9	5.9
Vapor Frac.:	0	0
Pressure:	2 atm	2 atm
Temperature:	80°F	212°F

Design Data:	Holdup Time:	0.167 hr	Pressure:	64.7 psig
	M.O.C.:	S.S	Temperature:	1700°F
	Length:	2.98 m	Volume:	2.4 m^3
	Type:	Mixing Tank	Diameter:	1 m
	Storage Material:	Salt Mix	Utility Flow:	2701 lbm/hr
	Utility Type:	LPS		

Vessels

Identification:	Item	Vessel		**Date:**	3/9/2017
	Item No.	V-101		**By:**	4287
	No. Required	1			

Function: Store well mixed salt solution prior to introduction into reactor

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	29566.5	29566.5
Component Flow:		
Water	17734	17734
Nylon-6,6	0	0
HMDA	5262.8	5262.8
Adipic Acid	6563.7	6563.7
N2O	5.9	5.9
Vapor Frac.:	0	0
Pressure:	2 atm	2 atm
Temperature:	212°F	212°F

Design Data:	Holdup Time:	0.167 hr	Pressure:	64.7 psig
	M.O.C.:	S.S.	Temperature:	1700°F
	Length:	3.1 m	Volume:	2.64 m^3
	Type:	Storage	Diameter:	1 m
	Storage Material:	Salt Mix		

Vessels

Identification:	Item	Flash Tank	**Date:**	3/9/2017
	Item No.	V-102	**By:**	4287
	No. Required	1		

Function: Remove water from the process to meet final product purity specifications

Operation: Standard

Materials Handled:	Inlet	Liq. Outlet	Vap. Outlet
Quantity (lb/hr)	10270.2	10226.1	44.1
Component Flow:			
Water	55.3	11.4	43.9
Nylon-6,6	10213.9	10213.9	0
HMDA	0.8	0.6	0.2
Adipic Acid	0.2	0.2	0
N2O	0	0	0
Pressure:	5 atm	1 atm	1 atm
Temperature:	550.5°F	540°F	540°F

Design Data:	Diameter:	2.7 m	Pressure:	50 psig
	M.O.C.:	S.S	Temperature:	1700°F
	Length:	8 m	Volume:	45.7 m^3
	Type:	Phase Separator	Hold Up:	0.083 hr

Vessels

Identification:	Item	Storage		**Date:**	3/9/2017
	Item No.	V-103		**By:**	4287
	No. Required	1			

Function: Emergency storage tank to hold molten nylon in case of extruder shutdown

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	10226.1
Component Flow:	
Water	11.4
Nylon-6,6	10213.9
HMDA	0.6
Adipic Acid	0.2
N2O	0
Pressure:	5 atm
Temperature:	540°F

Design Data:				
	Holdup Time:	24 hr	Pressure:	100 psig
	M.O.C.:	S.S.	Temperature:	1700°F
	Length:	11.4 m	Volume:	129 m^3
	Type:	Emergency	Diameter:	3.8 m
	Storage Material:	Molten Nylon		

Tanks

Identification:	Item	Storage	**Date:**	3/9/2017
	Item No.	T-100	**By:**	4287
	No. Required	1		

Function: Store process reactants

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	7518.3
Component Flow:	
Water	2255.5
Nylon-6,6	0
HMDA	5262.8
Adipic Acid	0
N2O	0
Pressure:	1 atm
Temperature:	80°F

Design Data:	Holdup Time:	30 days	Volume:	2027.6 m^3
	Type:	API Fixed Roof	Storage Material:	HMDA/Water

Tanks

Identification:	Item	Storage	**Date:**	3/9/2017
	Item No.	T-101	**By:**	4287
	No. Required	1		

Function: Store process reactants

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	6569.58
Component Flow:	
Water	0
Nylon-6,6	0
HMDA	0
Adipic Acid	6563.67
N2O	5.91
Pressure:	1 atm
Temperature:	80°F

Design Data:	Holdup Time:	30 days	Volume:	1576.2 m^3
	Type:	API Fixed Roof	Storage Material:	ADA

Tanks

Identification:	Item	Storage	**Date:**	3/9/2017
	Item No.	T-102	**By:**	4287
	No. Required	1		

Function: Store process reactants

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	15478.5
Component Flow:	
Water	15478.5
Nylon-6,6	0
HMDA	0
Adipic Acid	0
N2O	0
Pressure:	1 atm
Temperature:	80°F

Design Data:	Holdup Time:	30 days	Volume:	5791.7 m^3
	Type:	API Fixed Roof	Storage Material:	Water

Tanks

Identification:	Item	Storage	**Date:**	3/9/2017
	Item No.	T-103	**By:**	4287
	No. Required	3		

Function: Store process product, pelletized nylon-6,6 polymer

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	10226.1
Component Flow:	
Water	11.4
Nylon-6,6	10213.9
HMDA	0.6
Adipic Acid	0.2
N2O	0
Pressure:	1 atm
Temperature:	200°F

Design Data:	Holdup Time:	30 days	Volume:	3881.9 m^3
	Type:	API Fixed Roof	Storage Material:	Nylon Pellets

Screen

Identification:	Item	Pellet Screen	**Date:**	3/9/2017
	Item No.	S-100	**By:**	4287
	No. Required	3		

Function: Sift through formed pellets and eliminate off-spec sized product

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	10226.1	10226.1
Component Flow:		
Water	11.4	11.4
Nylon-6,6	10213.9	10213.9
HMDA	0.6	0.6
Adipic Acid	0.2	0.2
N2O	0	0
Pressure:	1 atm	1 atm
Temperature:	200°F	200°F

Design Data:	Type:	Vibrating	Pressure:	1 atm
	Area:	15 m^2	Temperature:	200°F

Conveyor

Identification:	Item	Conveyor	**Date:**	3/9/2017
	Item No.	Cv-100	**By:**	4287
	No. Required	1		

Function: Transport solid ADA to salt mixing tank

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (ft^3/hr)	77.3	77.3
Composition:		
Water	0	0
Nylon-6,6	0	0
HMDA	0	0
Adipic Acid	77.3	77.3
N2O	0	0
Pressure:	1 atm	1 atm
Temperature:	80°F	80°F

Design Data:	Type:	Belt	Width:	2 m
	Area:	55.7 m^2	Length:	300 m

Chute

Identification:	Item	Auto Chute	**Date:**	3/9/2017
	Item No.	Ch-100	**By:**	4287
	No. Required	1		

Function: Transport solid ADA to salt mixing tank

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (ft^3/hr)	77.3	77.3
Composition:		
Water	0	0
Nylon-6,6	0	0
HMDA	0	0
Adipic Acid	77.3	77.3
N2O	0	0
Pressure:	1 atm	1 atm
Temperature:	80°F	80°F

Design Data:				
	Inner Diameter:	3 ft	Heigth:	1 ft
	Volume:	6.44 ft^3	Hold-Up:	5 minutes
	M.O.C:	S.S.		

Extruder

Identification:	Item	Pelletizer	**Date:**	3/9/2017
	Item No.	X-100	**By:**	4287
	No. Required	5		

Function: Extrude molten nylon-6,6 and pelletize the product

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	10226.1	10226.1
Component Flow:		
Water	11.4	11.4
Nylon-6,6	10213.9	10213.9
HMDA	0.6	0.6
Adipic Acid	0.2	0.2
N2O	0	0
Pressure:	5 atm	1 atm
Temperature:	540°F	200°F

Design Data:	Type:	Double Screw	Screw Size:	8 in
	RPM:	100	L/D:	30
	Capacity:	1000 kg/hr		

Scrubber

Identification:	Item	Scrubber	**Date:**	3/9/2017
	Item No.	Sc-100	**By:**	4287
	No. Required	1		

Function: Remove Nitrous Oxide from water streams, waste treatment

Operation: Standard

Materials Handled:	
Quantity (kg/hr)	19340.4
Component Flow:	
Water	19325.47
Nitrous	5.92
Oxide	8.97
HMDA	0.29
Adipic Acid	3 atm
Pressure:	600°F

Design Data:	Heat Duty:	9.62E+7 Btu/hr	Type:	LNB + FGR

Reactor

Identification:	Item	Plug-Flow Rx	**Date:**	3/9/2017
	Item No.	R-200	**By:**	4287
	No. Required	1		

Function: Carry out the salt formation reactions associated with the formation of nylon-6,6

Operation: Standard

Materials Handled:	Feed (Liquid)	Mixed Prod.
Quantity (lb/hr)	29771	29771
Component Flow:		
Water	17857	19464
Nylon-6,6	0	10219
HMDA	5299.3	79.5
Adipic Acid	6609.2	3.5
N2O	6	6
Pressure:	5 atm	6 atm
Temperature:	233.6°F	530°F

Design Data:	Volume:	1256.9 ft^3	Pressure:	123.5 psig
	Length:	132.3 ft	Heat Duty:	2.93e+6 Btu/hr
	Diameter:	3.5 ft	Vapor Phase:	0.95
	M.O.C:	S.S	Liquid Phase:	0.05
	Residence Time:	.01 hr	Temperature:	1700°F
	Cycle Time:	N/A	Utility Type:	Paratherm HT
	Reaction:	Salt Formation		

Reactor

Identification:	Item	CSTR Reactor	**Date:**	3/9/2017
	Item No.	R-201	**By:**	4287
	No. Required	1		

Function: Carry out the polycondensation reaction in the formation of nylon-6,6

Operation: Standard

Materials Handled:	Feed (Liquid)	Liquid Prod.	Vapor Prod.
Quantity (lb/hr)	10259	10239	19.8
Component Flow:			
Water	37.8	24.8	19.8
Nylon-6,6	10219	10213.9	0
HMDA	1.5	0.06	0.005
Adipic Acid	1.1	0.6	0.002
N2O	0.003	0.0005	0.002
Pressure:	3 atm	2 atm	2 atm
Temperature:	530°F	530°F	530°F

Design Data:	Volume:	64 ft^3	Pressure:	64.7 psig
	Length:	4.4 ft	Heat Duty:	2.1e+4 Btu/hr
	Diameter:	4.4 ft	Vapor Phase:	0.002
	M.O.C:	S.S	Liquid Phase:	0.998
	Residence Time:	0.11 hr	Temperature:	1700°F
	Cycle Time:	N/A	Utility Type:	Paratherm HT
	Reaction:	Polycondensation		

Furnace

Identification:	Item	Fired Heater	**Date:**	3/9/2017
	Item No.	H-200	**By:**	4287
	No. Required	1		

Function: Heat reactor to specified temperature to induce step-growth reaction

Operation: Standard

Materials Handled:

Quantity (kg/hr)	47195.4
Component Flow:	
Paratherm HT	44374.8
Air	155
Natural Gas	2665.6
Pressure:	5 atm
Temperature:	600°F

Design Data:

Heat Duty: 7741.18 MJ/hr		U_o: 10 Btu/hr°Fft^2
Efficiency: 40%		Desired Temp: 550°F
M.O.C.: S.S		Utility Temp: 600°F
Coil Area: 1762 ft^2		

Furnace

Identification:	Item	Fired Heater	**Date:**	3/9/2017
	Item No.	H-201	**By:**	4287
	No. Required	1		

Function: Heat reactor to specified temperature to induce step-growth reaction

Operation: Standard

Materials Handled:

Quantity (kg/hr)	337.6
Component Flow:	
Paratherm HT	317.5
Air	1.1
Natural Gas	19
Pressure:	5 atm
Temperature:	600°F

Design Data:

Heat Duty: 55.4MJ/hr		U_o: 10 Btu/hr°Fft^2
Efficiency: 40%		Desired Temp: 550°F
M.O.C.: S.S		Utility Temp: 600°F
Coil Area: 39.2 ft^2		

Pump

Identification:	Item	Recip.		**Date:**	3/9/2017
	Item No.	P-200		**By:**	4287
	No. Required	2			

Function: Pump HMDA from storage to heated mixing tank V-100

Operation: Standard

Materials Handled:	Suction	Discharge
Quantity (lb/hr)	7570.4	7570.4
Component Flow:		
Water	2271.1	2271.1
Nylon-6,6	0	0
HMDA	5299.3	5299.3
Adipic Acid	0	0
N2O	0	0
Pressure:	1 atm	2 atm
Temperature:	80°F	82°F

Design Data:				
	Shaft Power:	0.152 kW	Pressure:	64.7 psig
	Pressure Ratio:	2	Temperature:	1100°F
	Delta P:	1 atm	Process Material:	HMDA/Water
	M.O.C:	Titanium		

Pump

Identification:	Item	Centrifugal	**Date:**	3/9/2017
	Item No.	P-201	**By:**	4287
	No. Required	2		

Function: Pump Deionized water from storage to heated mixing tank

Operation: Standard

Materials Handled:	Suction	Discharge
Quantity (lb/hr)	15586	15586
Component flows:		
Water	15586	15586
Nylon-6,6	0	0
HMDA	0	0
Adipic Acid	0	0
N2O	0	0
Pressure:	1 atm	2 atm
Temperature:	80°F	82°F

Design Data:	Shaft Power:	0.2531 kW	Pressure:	64.7 psig
	Pressure Ratio:	2	Temperature:	1400°F
	Delta P:	1 atm	Process Material:	Water
	M.O.C:	C.S		

Pump

Identification:	Item	Centrifugal	**Date:**	3/9/2017
	Item No.	P-202	**By:**	4287
	No. Required	2		

Function: Increase pressure from salt storage to transfer to reactor

Operation: Standard

Materials Handled:	Suction	Discharge
Quantity (lb/hr)	29771	29771
Component Flow:		
Water	17857	17857
Nylon-6,6	0	0
HMDA	5299.3	5299.3
Adipic Acid	6609.2	6609.2
N2O	5.95	5.95
Pressure:	2 atm	5 atm
Temperature:	210°F	212°F

Design Data:	Shaft Power:	1.662 kW	Pressure:	108.8 psig
	Pressure Ratio:	2.5	Temperature:	1700°F
	Delta P:	3 atm	Process Material:	Salt Mix
	M.O.C:	S.S		

Pump

Identification:	Item	Pos. Displace	**Date:**	3/9/2017
	Item No.	P-203	**By:**	4287
	No. Required	3		

Function: Pump molten nylon-6,6 product to densification and extrusion process

Operation: Standard

Materials Handled:	Suction	Discharge
Quantity (lb/hr)	10239	10239
Component Flow:		
Water	24.8	24.8
Nylon-6,6	10213.9	10213.9
HMDA	0.06	0.06
Adipic Acid	0.6	0.6
N2O	0.0005	0.0005
Pressure:	2 atm	5 atm
Temperature:	530°F	530.7°F

Design Data:				
	Shaft Power:	0.1147 kW	Pressure:	108.8 psig
	Pressure Ratio:	2.5	Temperature:	1700°F
	Delta P:	3 atm	Process Material:	Molten Nylon
	M.O.C:	S.S.		

Mixer

Identification:	Item	Tank Mixer	**Date:**	3/9/2017
	Item No.	M-200	**By:**	4287
	No. Required	2		

Function: Ensure contents of salt tank are well mixed prior to feeding into reactor

Operation: Standard

Materials Handled:

Quantity (lb/hr)	29771
Component Flow:	
Water	17857
Nylon-6,6	0
HMDA	5299.3
Adipic Acid	6609.2
N2O	5.95
Pressure:	2 atm
Temperature:	212°F

Design Data:	Shaft Power:	2.763 kW	Pressure:	2 atm
	M.O.C:	S.S	Temperature:	1700°F
	Process Material:	Salt Mix		

Heat Exchanger

Identification:	Item	S/T Fixed	**Date:**	3/9/2017
	Item No.	E-200	**By:**	4287
	No. Required	1		

Function: Pre-heat feed to reactor to ensure vapor-liquid interaction within reactor

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	14835	14835
Component Flow:		
Water	8898	8898
Nylon-6,6	0	0
HMDA	2640.6	2640.6
Adipic Acid	3293.4	3293.4
N2O	3	3
Vapor Frac.:	0	0
Pressure:	5 atm	5 atm
Temperature:	212°F	255°F

Design Data:				
	Heat Duty:	5.65e+5 Btu/hr	Pressure:	108.8 psig
	FEMA Type:	AES	Temperature:	1400°F
	M.O.C.:	S.S/C.S.	Utility Flow:	582.4 lbm/hr
	Delta P:	0	Utility Type:	LPS
	Utility Temp:	489.2°F	Utility Presure:	5 barg
	Approach Temp.:	20°F	Phase Change:	Shell Side
	Heat Transfer Area:	5.1 m^2	U_o:	40 Btu/hr°Fft^2
	Process Flow:	Salt Mix	Delta T:	35°F

Vessels

Identification:	Item	Salt Mixer		**Date:**	3/9/2017
	Item No.	V-200		**By:**	4287
	No. Required	1			

Function: Mix and Heat salt solution to 212 F prior to introduction into the reactor

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	29771	29771
Component Flow:		
Water	17857	17857
Nylon-6,6	0	0
HMDA	5299.3	5299.3
Adipic Acid	6609.2	6609.2
N2O	6	6
Vapor Frac.:	0	0
Pressure:	2 atm	2 atm
Temperature:	80°F	212°F

Design Data:				
	Holdup Time:	0.167 hr	Pressure:	64.7 psig
	M.O.C.:	S.S	Temperature:	1700°F
	Length:	3 m	Volume:	2.4 m^3
	Type:	Mixing Tank	Diameter:	1m
	Storage Material:	Salt Mix	Utility Flow:	2720.6 lbm/hr
	Utility Type:	LPS		

Vessels

Identification:	Item	Vessel	**Date:**	3/9/2017
	Item No.	V-201	**By:**	4287
	No. Required	1		

Function: Store well mixed salt solution prior to introduction into reactor

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	29771	29771
Component Flow:		
Water	17857	17857
Nylon-6,6	0	0
HMDA	5299.3	5299.3
Adipic Acid	6609.2	6609.2
N2O	6	6
Vapor Frac.:	0	0
Pressure:	2 atm	2 atm
Temperature:	212°F	212°F

Design Data:	Holdup Time:	0.167 hr	Pressure:	64.7 psig
	M.O.C.:	S.S.	Temperature:	1700°F
	Length:	3.1 m	Volume:	2.7 m^3
	Type:	Storage	Diameter:	1 m
	Storage Material:	Salt Mix		

Vessels

Identification:	Item	Flash Tank		**Date:**	3/9/2017
	Item No.	V-202		**By:**	4287
	No. Required	1			

Function: Remove water from the process to meet final product purity specifications

Operation: Standard

Materials Handled:	Inlet	Liq. Outlet	Vap. Outlet
Quantity (lb/hr)	29771	10259	19512
Component Flow:			
Water	19464	37.8	19426
Nylon-6,6	10219	10219	0
HMDA	79.5	1.5	78
Adipic Acid	3.5	1.1	2.4
N2O	6	0	6
Pressure:	6 atm	3 atm	3 atm
Temperature:	530°F	530°F	530°F

Design Data:	Diameter:	3.8 m	Pressure:	79.4 psig
	M.O.C.:	S.S	Temperature:	1700°F
	Length:	11.5 m	Volume:	132.3 m^3
	Type:	Phase Separator	Hold Up:	0.083 hr

Vessels

Identification:	Item	Storage		**Date:**	3/9/2017
	Item No.	V-203		**By:**	4287
	No. Required	1			

Function: Emergency storage tank to hold molten nylon in case of extruder shutdown

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	10239
Component Flow:	
Water	24.8
Nylon-6,6	10213.9
HMDA	0.06
Adipic Acid	0.6
N2O	0
Pressure:	5 atm
Temperature:	530.7°F

Design Data:				
	Holdup Time:	24 hr	Pressure:	100 psig
	M.O.C.:	S.S	Temperature:	1700°F
	Length:	11.4 m	Volume:	129 m^3
	Type:	Emergency	Diameter:	3.8 m
	Storage Material:	Molten Nylon		

Tanks

Identification:	Item	Storage	**Date:**	3/9/2017
	Item No.	T-200	**By:**	4287
	No. Required	1		

Function: Store process reactants

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	7570.4
Component Flow:	
Water	2271.1
Nylon-6,6	0
HMDA	5299.3
Adipic Acid	0
N2O	0
Pressure:	1 atm
Temperature:	80°F

Design Data:	Holdup Time:	30 days	Volume:	2041.6 m^3
	Type:	API Fixed Roof	Storage Material:	HMDA/Water

Tanks

Identification:	Item	Storage	**Date:**	3/9/2017
	Item No.	T-201	**By:**	4287
	No. Required	1		

Function: Store process reactants

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	6615.2
Component Flow:	
Water	0
Nylon-6,6	0
HMDA	0
Adipic Acid	6609.2
N2O	5.95
Pressure:	1 atm
Temperature:	80°F

Design Data:	Holdup Time:	30 days	Volume:	1587.1 m^3
	Type:	API Fixed Roof	Storage Material:	ADA

Tanks

Identification:	Item	Storage	**Date:**	3/9/2017
	Item No.	T-202	**By:**	4287
	No. Required	1		

Function: Store process reactants

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	15586
Component Flow:	
Water	15586
Nylon-6,6	0
HMDA	0
Adipic Acid	0
N2O	0
Pressure:	1 atm
Temperature:	80°F

Design Data:	Holdup Time:	30 days	Volume:	5831.8 m^3
	Type:	API Fixed Roof	Storage Material:	Water

Tanks

Identification:	Item	Storage	**Date:**	3/9/2017
	Item No.	T-203	**By:**	4287
	No. Required	3		

Function: Store process product, pelletized Nylon-6,6 polymer

Operation: Standard

Materials Handled:	Inlet
Quantity (lb/hr)	10239
Component Flow:	
Water	24.8
Nylon-6,6	10213.9
HMDA	0.06
Adipic Acid	0.6
N2O	0
Pressure:	1 atm
Temperature:	200°F

Design Data:	Holdup Time:	30 days	Volume:	3868.2 m^3
	Type:	API Fixed Roof	Storage Material:	Nylon Pellets

Screen

Identification:	Item	Pellet Screen	**Date:**	3/9/2017
	Item No.	S-200	**By:**	4287
	No. Required	3		

Function: Sift through formed pellets and eliminate off-spec sized product

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	10239	10239
Component Flow:		
Water	24.8	24.8
Nylon-6,6	10213.9	10213.9
HMDA	0.06	0.06
Adipic Acid	0.6	0.6
N2O	0.0005	0.0005
Pressure:	1 atm	1 atm
Temperature:	200°F	200°F

Design Data:	Type:	Vibrating	Pressure:	1 atm
	Area:	15 m^2	Temperature:	200°F

Conveyor

Identification:	Item	Conveyor	**Date:**	3/9/2017
	Item No.	Cv-200	**By:**	4287
	No. Required	1		

Function: Transport solid ADA to salt mixing tank

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (ft^3/hr)	77.8	77.8
Composition:		
Water	0	0
Nylon-6,6	0	0
HMDA	0	0
Adipic Acid	77.8	77.8
N2O	0	0
Pressure:	1 atm	1 atm
Temperature:	80°F	80°F

Design Data:	Type:	Belt	Width:	2 m
	Area:	55.7 m^2	Length:	300 m

Chute

Identification:	Item	Auto Chute	**Date:**	3/9/2017
	Item No.	Ch-200	**By:**	4287
	No. Required	1		

Function: Transport solid ADA to salt mixing tank

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (ft^3/hr)	77.8	77.8
Composition:		
Water	0	0
Nylon-6,6	0	0
HMDA	0	0
Adipic Acid	77.8	77.8
N2O	0	0
Pressure:	1 atm	1 atm
Temperature:	80°F	80°F

Design Data:

Inner Diameter: 3 ft

Heigth: 1 ft

Volume: 6.49 ft^3

Hold-Up: 5 minutes

M.O.C: S.S.

Extruder

Identification:	Item	Pelletizer	**Date:**	3/9/2017
	Item No.	X-200	**By:**	4287
	No. Required	5		

Function: Extrude molten nylon-6,6 and pelletize the product

Operation: Standard

Materials Handled:	Inlet	Outlet
Quantity (lb/hr)	10239	10239
Component Flow:		
Water	24.8	24.8
Nylon-6,6	10213.9	10213.9
HMDA	0.06	0.06
Adipic Acid	0.6	0.6
N2O	0.0005	0.0005
Pressure:	5 atm	1 atm
Temperature:	530.7°F	200°F

Design Data:

Type: Double Screw

Screw Size: 8 in

RPM: 100

L/D: 30

Capacity: 1000 kg/hr

Scrubber

Identification:	Item	Scrubber	**Date:**	3/9/2017
	Item No.	Sc-200	**By:**	4287
	No. Required	1		
Function:	Remove Nitrous Oxide from water streams, waste treatment			
Operation: Standard				

Materials Handled:	
Quantity (kg/hr)	19531.9
Component Flow:	
Water	19445.60
Nitrous Oxide	5.95
HMDA	77.95
Adipic	2.38
Acid	3 atm
Pressure:	600°F

Design Data:	Heat Duty: 9.62E+7 Btu/hr	Type: LNB + FGR

Equipment Cost Summary

In the process design, the group encountered a few issues with costing equipment by size. Table 13 below summarizes each piece of equipment that required assumptions or encountered issues in the batch design process.

Table 13. Batch Process Design Assumptions/Issues with Costing

Batch Process Design	
Equipment Description	**Assumptions / Issues**
Hot Oil Heat Exchanger	The heat transfer area is too large for the costing correlations. The exchanger was costed as two exchangers in series.
Salt Mixer	The required power is too small for the costing correlations. The smallest power that made the correlation valid was used, 5 kW.
Pre-Feed Heat Exchanger	The heat transfer area is too small for the costing correlations. The smallest heat exchanger area that made the correlation valid was used, 10 square meters.

HMDA Pump	The required shaft power is too small for the costing correlations. The smallest shaft power that made the correlation valid was used, 1 kW.
Water Pump	The required shaft power is too small for the costing correlations. The smallest shaft power that made the correlation valid was used, 1 kW.

The following table lists the equipment that required assumptions or encountered issues in the sizing of the continuous process design.

Table 14. Continuous Process Design Assumptions/Issues with Costing

Continuous Process Design	
Equipment Description	**Assumptions / Issues**
CSTR Heat Exchanger	The heat transfer area is too small for the costing correlations. The smallest heat exchanger area that made the correlation valid was used, 10 square meters.
CSTR Furnace	The required furnace duty is too small for the costing correlations. The furnace was costed using the smallest heat duty that made the correlation valid, 3600 MJ per hour.
CSTR Mixer	The required power is too small for the costing correlations. The smallest power that made the correlation valid was used, 5 kW.
Salt Mixer	The required power is too small for the costing correlations. The smallest power that made the correlation valid was used, 5 kW.
Pre-Feed Heat Exchanger	The heat transfer area is too small for the costing correlations. The smallest heat exchanger area that made the correlation valid was used, 10 square meters.
HMDA Pump	The required shaft power is too small for the costing correlations. The smallest shaft power that made the correlation valid was used, 1 kW.

Water Pump	The required shaft power is too small for the costing correlations. The smallest shaft power that made the correlation valid was used, 1 kW.

The capital costs for the batch design process are outlined in Table 15 below. The equipment number and description are given with the grass roots cost for the process.

Table 15. Equipment Grass Roots Cost for Batch Process

Equipment Number	Equipment Description	Grass Roots Cost for Quantity Needed (USD)
R-100	Batch Reactor Vessel	$1,100,000
	Batch Reactor CW HEX	$200,000
	Batch Reactor Hot Oil HEX	$6,100,000
H-100	Batch Reactor Furnace	$6,800,000
P-100	HMDA Pump	$266,000
P-101	Water Pump	$42,000
P-102	Nylon Salt Pump	$52,000
P-103	Nylon-6,6 Pump	$100,000
M-100	Stirred Mixer	$150,000
E-100	Pre-Feed HEX	$150,000
V-100	Stirred Vessel HEX	$150,000
	Stirred Vessel	$74,000
V-101	Nylon Salt Storage Tank	$80,000
V-102	Flash Tank	$730,000
V-103	Emergency Molten Storage Tank	$2,100,000
T-101	ADA Storage Tank	$290,000
T-100	HMDA Storage Tank	$330,000
T-102	Water Storage Tank	$630,000
T-103	Nylon-6,6 Storage Tank	$490,000
S-100	Pellet Screens	$360,000
Cv-100	ADA Conveyor	$260,000
Ch-100	ADA Chute	$1,800
X-100	Extruder	$170,000

Sc-100	N2O Scrubber	$210,000
Total Capital Cost for Batch Process		**$21,000,000**

The capital costs for each piece of equipment in the continuous process design are outlined in the following table.

Table 16. Equipment Grass Roots Cost for Continuous Process

Equipment Number	Equipment Description	Grass Roots Cost for Quantity Needed (USD)
R-200	PFR Vessel	$460,000
	PFR HEX	$320,000
R-201	CSTR Vessel	$72,000
	CSTR HEX	$190,000
	CSTR Mixer	$130,000
H-200	PFR Furnace	$3,100,000
H-201	CSTR Furnace	$2,800,000
P-200	HMDA Pump	$266,000
P-201	Water Pump	$42,000
P-202	Nylon Salt Pump	$52,000
P-203	Nylon-6,6 Pump	$100,000
M-200	Stirred Mixer	$130,000
E-200	Pre-Feed HEX	$150,000
V-200	Stirred Vessel HEX	$150,000
	Stirred Vessel	$75,000
V-201	Nylon Salt Storage Tank	$80,000
V-202	Flash Tank	$2,800,000
V-203	Emergency Molten Storage Tank	$2,400,000
T-201	ADA Storage Tank	$290,000
T-200	HMDA Storage Tank	$330,000
T-202	Water Storage Tank	$640,000
T-203	Nylon-6,6 Storage Tank	$490,000
S-200	Pellet Screens	$360,000
Cv-200	ADA Conveyor	$260,000
Ch-200	ADA Chute	$1,800

X-200	Extruder	$170,000
Sc-200	N2O Scrubber	$210,000
Total Capital Cost for Continuous Process		**$16,000,000**

As shown from the comparison between Tables 15 and 16, the continuous process has a lower total capital cost than the batch design process.

Fixed Capital Investment Summary

Costing Correlations

The capital cost for each piece of equipment can be seen in the Equipment Cost Summary section above. The CapCOST program published by Turton et al. was used to calculate purchase, installation, total module, and grass roots costs for every piece of equipment with the exception of the ADA Chute, Extruder, and N_2O Scrubber[62]. The ADA Chute, Extruder and Scrubber were costed based on information found in additional sources[36][39][63]. Equations (18) to (27) represent the equations used by the CapCOST program to calculate the equipment costs.

Equations (18) to (20) below list all the general equations used to calculated the purchase costs. Note that all variables are defined in Appendix Table A1.

$$log_{10}C_p^0 = K_1 + K_2 log_{10}(A) + K_3[log_{10}(A)]^2 \tag{18}$$

$$F_p = \left[\frac{\left(\frac{(P+1)D}{2[850-0.6(P+1)]}\right) + 0.00315}{0.0063}\right] \tag{19}$$

$$log_{10}F_p = C_1 + C_2 log_{10}(P) + C_3[log_{10}(P)]^2 \tag{20}$$

Equations (21) to (24) below list all the general equations used to calculate the installation costs.

$$C_{BM} = C_p^0 F_{BM} \tag{21}$$

$$C_{BM} = C_p^0 F_{BM} F_P F_T \tag{22}$$

$$F_{BM} = (B_1 + B_2 F_m F_p) \tag{23}$$

$$F_T = 1 \tag{24}$$

Equation (25) below was used to calculate the total module cost. This accounts for 15% contingency and 3% fees.

$$C_{TM} = 1.18(C_{BM}) \tag{25}$$

Equations (26) and (27) below list all the general equations used to calculate the grass-roots costs.

$$C_{GR} = C_{TM} + 0.5C_{BM}^0 \tag{26}$$

$$C_{BM}^0 = C_{BM} \text{ evaluated at base conditions} \tag{27}$$
(ambient pressure, carbon steel equipment)

In Equations (19) and (20), the pressure used was the design pressure which was calculated using Equation (28).

$$P = P_{Aspen} + 50\ psi \tag{28}$$

Once CapCOST generated the grass-roots costs for each piece of equipment, the grass-roots costs were multiplied by a CEPCI factor of (540.9/397) to escalate costs to June 2016[62]. The CapCOST software calculations were validated by hand calculations for the salt mixer costs shown in Appendix Table A110.

The cost calculation equations and parameters used for each piece of equipment are in the itemized sections below.

Batch Reactor: R-100

The batch reactor cost was calculated as the summation of a vertical vessel, a cooling water heat exchanger, and a hot oil heat exchanger[66]. Equation (18) was used to calculate the purchase cost. The parameters for this equation are shown in Table 17 below.

Table 17. Parameters for Equation 18 for R-100

Parameter	Vessel	Heat Exchanger
Equipment Description	Vertical	Shell and Tube
K1	3.4974	4.3247
K2	0.4485	-0.303

K3	0.1074	0.1634
A	Volume, m^3	Area, m^2

The volume of the batch reactor was calculated utilizing Equation (29).

$$V_{batch} = \frac{f_b(t_{feed})}{0.6} \tag{29}$$

The area of the heat exchanger was calculated utilizing Equation (30). The hot oil heat exchanger was too large to cost with the given correlation, so it was costed as two heat exchangers in series.

$$A = \frac{Q}{U\Delta T_{lm}} \tag{30}$$

The log mean temperature difference was calculated utilizing Equation (31).

$$\Delta T_{lm} = \frac{\left(T_{H,in} - T_{C,out}\right) - \left(T_{H,out} - T_{C,in}\right)}{\ln(\left(T_{H,in} - T_{C,out}\right) - \left(T_{H,out} - T_{C,in}\right))} \tag{31}$$

Equation (21) was used to calculate the installation cost for both the vessel and the heat exchanger. The bare module factor for the mixer was a constant value of 1.38. In order to calculate the installation cost for the vessel and the heat exchanger, the pressure factor and bare module factor had to be determined. Table 18 details the equations and parameters used to determine the values of these factors.

Table 18. Factors Used to Calculate Installed Cost for R-100

Factor	Vessel	Cooling Water Heat Exchanger	Hot Oil Heat Exchanger
Pressure Factor	Equation (19)	Equation (20) C1 = 0.03881 C2 = -0.11272 C3 = 0.08183	Equation (20) C1 = 0.03881 C2 = -0.11272 C3 = 0.08183
Bare Module Factor	Equation (23) B1 = 2.25 B2 = 1.82 Fm = 3.1	Equation (23) B1 = 1.63 B2 = 1.66 Fm = 1.81	Equation (23) B1 = 1.63 B2 = 1.66 Fm = 2.73

Plug Flow Reactor: R-200

The plug flow reactor cost was calculated as the summation of two horizontal vessels and a heat exchanger[66]. Equation (18) was used to calculate the purchase cost. The parameters for this equation are shown in Table 19 below.

Table 19. Parameters for Equation 18 for R-200

Parameter	Vessel	Heat Exchanger
Equipment Description	Horizontal	Shell and Tube
K1	3.5565	4.3247
K2	0.3776	-0.303
K3	0.0905	0.1634
A	Volume, m^3	Area, m^2

The volume of the vessel was taken from Aspen Plus after optimization of the design. The area of the heat exchanger was calculated utilizing Equations (30) and (31) in the batch section above. The heat duty and cold temperatures were also taken from Aspen Plus. The supply temperature of the hot oil was determined by the maximum value that the Paratherm HT was rated for[46]. An approach temperature of 20 °F was assumed.

Equation (21) was used to calculate the installation cost for both the vessel and the heat exchanger. In order to calculate the installation cost, the pressure factor and bare module factor had to be determined. Table 20 details the equations and parameters used to determine the values of these factors.

Table 20. Factors used to Calculate Installed Cost for R-200

Factor	Vessel	Heat Exchanger
Pressure Factor	Equation (19)	Equation (20) C1 = 0.03881 C2 = -0.11272 C3 = 0.08183
Bare Module Factor	Equation (23) B1 = 1.49 B2 = 1.52 Fm = 3.1	Equation (23) B1 = 1.63 B2 = 1.66 Fm = 2.73

Continuous Stirred Tank Reactor: R-201

The continuous stirred tank reactor cost was calculated as the summation of a vertical vessel, heat exchanger, and mixer[66]. Equation(18) was used to calculate the purchase cost. The parameters for this equation are shown in Table 21 below.

Table 21. Parameters for Equation 18 for R-201

Parameter	Vessel	Heat Exchanger	Mixer
Equipment Description	Vertical	Shell and Tube	Propeller
K1	3.4974	4.3247	4.3207
K2	0.4485	-0.303	0.0356
K3	0.1074	0.1634	0.1346
A	Volume, m^3	Area, m^2	Power, kW

The volume of the CSTR was calculated utilizing Equation (32).

$$V_{CSTR} = \frac{f_{in} t_{holdup}}{0.6} \tag{32}$$

The area of the heat exchanger was calculated utilizing Equations (30) and (31) shown above in the batch section. The duty provided by Aspen Plus was the net duty of the reactor. As such, any negative and positive values of the duty were summed resulting in a small positive duty. The area calculated with this duty was too small and the capital cost was calculated with the minimum area of 10 m^2.

The power of the mixer was calculated by simulating a pump in Aspen HYSYS that doubled the inlet pressure. The value of the power was then pulled from Aspen HYSYS. The resulting power from this method, however, was too small and the capital cost was calculated with the minimum value of 5 kW.

Equation (21) was used to calculate the installation cost for the vessel, the heat exchanger, and the mixer. The bare module factor for the mixer was a constant value of 1.38. In order to calculate the installation cost for the vessel and the heat exchanger, the pressure factor and bare module factor had to be determined. Table 22 details the equations and parameters used to determine the values of these factors.

Table 22. Factors used to Calculate Installed Cost for R-201

Factor	Vessel	Heat Exchanger
Pressure Factor	Equation (19)	Equation (20) C1 = 0.03881 C2 = -0.11272 C3 = 0.08183
Bare Module Factor	Equation (23) B1 = 2.25 B2 = 1.82 Fm = 3.1	Equation (23) B1 = 1.63 B2 = 1.66 Fm = 2.73

Furnace: H-100, H-200, H-201

For the PFR, CSTR, and batch reactor, a furnace was used to heat Paratherm HT to elevate the temperature to the desired set point. The parameters were the same for all the furnaces. Equation (18) was used to calculate the purchase cost. The parameters for this equation are shown below in Table 23.

Table 23. Parameters for Equation 18 for Furnaces

Parameter	Fired Heater
Equipment Description	Process Heater
K1	7.3488
K2	-1.1666
K3	0.2028
A	Duty, MJ/hr

For the CSTR furnace, the duty was too small so the cost was evaluated at the minimum duty of 3600 MJ/hr. For the batch and PFR, the duty was taken from Aspen Plus reactor profiles.

Equation (22) was used to calculate the installation cost. In order to calculate this value, the bare module factor, temperature factor, and pressure factor were determined. The bare module factor was a constant value of 2.81. The temperature factor was 1 as shown in Equation (24). The pressure factor was calculated using Equation (20). The parameters used in this equation are shown in Table 24.

Table 24. Parameters for Equation 20 for Furnaces

Factor	Fired Heater
C1	0.1347
C2	-0.2368
C3	0.09403

Pumps: P-100, P-101, P-102, P-103, P-200, P-201, P-202, P-203

The deionized water and nylon salt pumps were costed as centrifugal pumps. The HMDA pump was costed as a reciprocating pump. The molten nylon-6,6 pump was costed as a positive displacement pump. The purchase cost for each of these pumps was calculated utilizing Equation (18). The parameters used for the different types of pumps in this equation are detailed in Table 25 below.

Table 25. Parameters for Equation 18 for Pumps

Parameter	Centrifugal Pumps	Reciprocating Pump	Positive Displacement Pump
K1	3.3892	3.8696	3.4771
K2	0.0536	0.3161	0.1350
K3	0.1538	0.1221	0.14380
A	Power, kW	Power, kW	Power, kW

The power for each of these pumps was determined by simulating the flow streams in Aspen HYSYS. For the nylon-6,6 pump, a mixture of mercury and water was used to simulate the same density and process flow conditions at that point in the process as Aspen HYSYS does not have polymers enabled.

The installation cost was calculated utilizing equation (21). In order to calculate this cost, the pressure factor, material factor, and bare module factor had to be determined. Table 26 details the equations and parameters used to determine the values of these factors for each pump.

Table 26. Factors to Calculate Installed Cost for Pumps

Factor	HMDA Pump	Deionized Water Pump	Nylon Salt Pump	Molten Nylon 6,6 Pump
Pressure Factor	Equation (20)			
C1	-0.245382	-0.3935	-0.3935	-0.24538
C2	0.259016	0.3957	0.3957	0.259016
C3	-0.01363	-0.00226	-0.00226	-0.01363
Bare Module Factor	Equation (23)			
B1	1.89	1.89	1.89	1.89
B2	1.35	1.35	1.35	1.35
Fm	6.4	1.6	2.3	2.7

Nylon Salt Mixer: V-100, V-200, M-100, M-200

The nylon salt mixer cost was calculated as the summation of a vertical vessel, heat exchanger, and mixer. Equation (18) was used to calculate the purchase cost. The parameters for this equation are shown in Table 27 below.

Table 27. Parameters for Equation 18 for Nylon Salt Mixer

Parameter	Vessel	Heat Exchanger	Mixer
Equipment Description	Vertical	Shell and Tube	Propeller
K1	3.4974	4.3247	3.8511
K2	0.4485	-0.303	0.07009
K3	0.1074	0.1634	-0.0003
A	Volume, m^3	Area, m^2	Power, kW

The volume of the vessel was calculated utilizing Equation (33). A holdup time of 10 minutes was used per heuristics[62].

$$V_i = f_{in,i} t_{holdup,i} \tag{33}$$

The heat exchanger area was calculated utilizing Equations (30) and (31) in the batch section above.

The power of the mixer was calculated by simulating a pump in Aspen HYSYS that doubled the inlet pressure. The value of the power was then pulled from Aspen

HYSYS. The resulting power from this method, however, was too small and the capital cost was calculated with the minimum value of 5 kW.

Equation (21) was used to calculate the installation cost for the vessel, the heat exchanger, and the mixer. The bare module factor for the mixer was a constant value of 1.38. In order to calculate the installation cost for the vessel and the heat exchanger, the pressure factor and bare module factor had to be determined. Table 28 details the equations and parameters used to determine the values of these factors.

Table 28. Factors to Calculate Installed Cost for Nylon Salt Mixer

Factor	Vessel	Heat Exchanger
Pressure Factor	Equation (19)	Equation (20) C1 = 0.03881 C2 = -0.11272 C3 = 0.08183
Bare Module Factor	Equation (23) B1 = 2.25 B2 = 1.82 Fm = 3.1	Equation (23) B1 = 1.63 B2 = 1.66 Fm = 1.81

Pre-Feed Heat Exchanger: E-100, E-200

The pre-feed heat exchanger purchase cost was calculated utilizing Equation (18). The parameters for this equation are shown in Table 29 below.

Table 29. Parameters for Equation 18 for Pre-Feed Heat Exchangers

Parameter	Heat Exchanger
Equipment Description	Shell and Tube
K1	4.3247
K2	-0.303
K3	0.1634
A	Area, m^2

The heat exchanger area of the pre-feed heat exchanger was calculated utilizing Equations (30) and (31) in the batch section above. The utility temperature of the low pressure steam was a heuristic value[62]. An approach temperature of 20 °F was assumed.

Equation (21) was used to calculate the installation cost for the heat exchanger. In order to calculate the bare module cost for the heat exchanger, the pressure factor and bare module factor had to be determined. Table 30 details the equations and parameters used to determine the values of these factors.

Table 30. Factors to Calculate Installed Cost for Pre-Feed Heat Exchangers

Factor	Heat Exchanger
Pressure Factor	Equation (20)
C1	0.03881
C2	-0.11272
C3	0.08183
Bare Module Factor	Equation (23)
B1	1.63
B2	1.66
Fm	1.81

Process Vessels: V-101, V-102, V-103, V-201, V-202, V-203

The flash tank, nylon salt storage tank, and emergency molten storage vessel purchase costs were calculated utilizing Equation (18). The parameters for this equation are shown in Table 31 below.

Table 31. Parameters for Equation 18 for Process Vessels

Parameter	Flash Tank
Equipment Description	Vertical Vessel
K1	3.4974
K2	0.4485
K3	0.1074
A	Volume, m^3

The volumes of the flash tank and nylon salt storage tank were calculated utilizing Equation (33) in the salt mixer storage tank section above. The holdup time for the flash tank was 6 minutes according to heuristics[62]. The holdup time for the nylon salt storage tank was 10 minutes according to heuristics[62]. The holdup time for the emergency storage vessel was assumed to be 24 hours.

Equation (21) was used to calculate the installation cost for both the flash tank. In order to calculate the installation cost for the vessel, the pressure factor and bare module factor had to be determined. Table 32 details the equations and parameters used to determine the values of these factors.

Table 32. Factors to Calculate Installed Cost for Process Vessels

Factor	Vessel
Pressure Factor	Equation (19)
Bare Module Factor	Equation (23)
B1	2.25
B2	1.82
Fm	3.1

Tanks: T-100, T-101, T-102, T-103, T-200, T-201, T-202, T-203

The storage tanks for ADA, HMDA, deionized water, and nylon-6,6 were costed with the same parameters. Equation (18) was used to determine the purchase cost of the storage tanks. The parameters for this equation are shown below in Table 33.

Table 33. Parameters for Equation 18 for Tanks

Parameter	**Storage Tank**
Equipment Description	Fixed Roof
K1	4.8509
K2	-0.3973
K3	0.1445
A	Volume, m^3

The volume of the storage tanks were calculated utilizing Equation (34). The storage time for the tanks was 30 days according to heuristics[62].

$$V_i = f_{in,i} t_{store,i} \tag{34}$$

Equation (21) was used to calculate the installation cost. In order to calculate the bare module cost, the bare module factor was determined using Equation (23). The parameters for this equation are shown below in Table 34.

Table 34. Bare Module Factors for Tanks

Parameter	**Storage Tank**
Bare Module Factor	Fixed Roof
B1	1.10
B2	0

Pellet Screens: S-100, S-200

The pellet screen purchase cost was calculated utilizing Equation (18). The parameters for this equation are shown in Table 35 below.

Table 35. Parameters for Equation 18 for Pellet Screens

Parameter	**Conveyor**
Equipment Description	Vibrating
K1	4.0485
K2	0.1118
K3	0.3260
A	Area, m^2

The maximum area for the screen cost correlations was used for cost estimation.

The installation cost for the screen was calculated utilizing Equation (21). The bare module factor was a constant value of 1.34.

Conveyor: Cv-100, Cv-200

The conveyor purchase cost was calculated utilizing Equation (18). The parameters for this equation are shown below in Table 36.

Table 36. Parameters for Equation 18 for Conveyor

Parameter	Conveyor
Equipment Description	Belt
K1	4.0637
K2	0.2584
K3	0.1550
A	Area, m^2

The area of the conveyor belt was calculated based on the width and length of the belt which were determined based on the flow rate. A belt length of 100 feet one way was assumed. The width of the belt was then calculated using Equation (35)[65]. This width was then doubled to account for possible future increased capacity.

$$W_{belt} = \frac{m_{belt}}{\rho * l_{belt}} \tag{35}$$

The installation cost for the conveyor was calculated utilizing Equation (21). The bare module factor was a constant value of 1.25.

Chute

The grass-roots cost of the chute was calculated utilizing data from a miscellaneous industrial costing source[36]. The largest inside diameter for the chute was used to determine the cost per foot of height at $115.50[36]. A holdup time of 5 minutes was assumed based on heuristics[62]. This resulted in a height of one foot. A cost of $1,500 was added to the purchase cost to include electrically operated doors[36]. A factor of 1.25 was multiplied by the purchase cost to include the increased cost of a stainless steel chute[36].

Extruder: X-100, X-200

The extruder grass-roots cost was determined from a vendor price for an extruder[63]. The capacity required of the extruder and the capacity of the vendor supplied extruder was used to calculate that 5 extruders were needed. The grass-roots cost per extruder was then multiplied by the number of extruders to determine the total grass-roots cost for the extruders.

N_2O Scrubber

The N_2O scrubber was costed based on a rate of $54.24 in cost/kW of duty required to burn the N_2O[39]. The N2O scrubber was simulated in Aspen HYSYS and the duty required was pulled from the simulation.

Safety, Health, and Environmental Considerations

Reaction Components

The raw materials associated with nylon-6,6 production include HMDA, ADA, and deionized water. Both of the reacting components present inherent risks that have been taken into account during this preliminary process design. In addition to the risks associated with the reactants, nitrous oxide is introduced into the system, as well. Nitrous oxide is formed in the manufacturing process of ADA, and while many manufacturers are able to get rid of most of the N_2O prior to sale, the group chose to look at the effects of having this material introduced into the process of nylon-6,6 manufacturing[60]. The design solutions to maintain safety, health, and the environment with the use of the hazardous components will be discussed in the following paragraphs.

ADA and HMDA are both hazardous to humans and the group has taken this into account when designing the nylon-6,6 process[13][14]. Equipment has been designed to limit the amount of time spent by operators and other facility employees interacting with the process. In addition to designing the process to limit human contact with all components, the group has also developed a control strategy to further reduce human contact from the process equipment. The group designed a process to limit exposure of chemicals to the community surrounding the plant by keeping all chemicals enclosed, either in enclosed storage or within the piping, throughout the entire process.

ADA is most commonly a colorless, crystalline powder. The compound is a weak acid that is combustible and dust particles are explosive[13]. The group has designed the process to limit the risk of combustion by keeping open flames away from the ADA at all points in the process. The group also included an enclosed conveyor to transport the ADA to the beginning of the nylon-6,6 process. This precaution was initially proposed because of the potential for dust cloud explosion, but with the addition of an enclosed conveyor, the amount of dust particles that could be released into the environment has been limited. This is crucial to the safety of the community around the plant, as ADA dust can be harmful if inhaled[13]. The ADA storage is also sealed to the environment so that dust will not be released via this method.

HMDA is delivered to the process in the form of an aqueous solution. A major concern to the group is that HMDA is corrosive, therefore, all material in contact with HMDA is made of titanium. The group also recommends frequent checking of equipment in contact with HMDA to ensure no fatal corrosion has occurred[37]. HMDA will also react with oxidants and will react violently with strong acids so the exposure to these elements has been eliminated due to the storage design for the HMDA solutions[37]. The solution is also combustible and the vapors that can form when the solution is heated are explosive[37]. Again, the group has made design decisions to eliminate any contact of HMDA with open flames and high storage temperatures to lower this risk significantly.

While nitrous oxide itself is not combustible, it does enhance the combustion capabilities of other compounds[15]. Again, the group's decision to limit exposure to open flames is employed because of the potential of enhanced combustion of the other compounds. Another danger of N_2O is the fact that it is denser than air and can accumulate in low ceiling areas and deplete the oxygen concentration[15]. This will be avoided as the N_2O will always be in an enclosed area before it is eventually scrubbed from the process.

Process

There are several factors associated with the overall process of nylon-6,6 production that add risk units to the system. Not only are the reactants utilized corrosive, the reaction itself requires high temperatures. This is due to the rate constants associated with the step growth polymerization of nylon-6,6[17]. Additionally, due to the high melting point of the polymer the reaction must take place at a point that will allow the product to be molten liquid and can be easily pumped from one point in the process to the next[43]. These high temperatures pose serious personnel risk. To minimize the amount of probable exposure time with personnel the group has provided a preliminary control system design. This control system allows the units to operate at a safe distance away from personnel.

In order to combat the inherent risks with the system the group utilized several concepts to reduce the implicit risk within the process.

1. Minimization:

When comparing a batch or continuous process the design group recognized that with a continuous process, there is a decrease in inventory storage, which leads to an inherently safer design. Furthermore, the possibility of explosive clouds with ADA dust, led the group to design a contained conveyor system to minimize the chemicals contact with open atmosphere[2]. To eradicate the risk associated with recycle streams the design encompasses high conversion reactors that have no need for the recycling of reactants. This decreases the amount of intermediates present in the process lines.

2. Substitution:

During every step of the preliminary design process of the system, the group ensured that every piece of equipment was designed with the proper materials of construction. Due to the high temperatures, volatility of components, and sheer volume of process media the group elected to select MOCs that prove to be more than capable of containing the reactants and products formed. Additionally, the group notes that the design will have to utilize hot oils to heat the reactors to the necessary temperatures, in order to combat the risks associated with this heating media, all piping was designed to have sufficient insulation. This will need to be researched further in detailed design.

3. Moderation:

The compounds used in this reaction pose serious concern if utilized at concentrated amounts. In order to alleviate this, concern the group utilized mixing tanks to dilute the reactant solutions before they are introduced into the process lines. Furthermore, the reaction kinetics are heavily dependent on temperature, but not pressure. With this knowledge, the highest process pressure is 6 atm, this allows the system to avoid high pressures, and consequently reduces risk.

4. Simplification:

While designing the overall process the group was diligent in looking for pieces of equipment that could be combined in order to reduce the total number of units needed to be monitored by operators. With this in mind, the group elected to utilize the CSTR that is downstream of the PFR in the continuous process as a condensation reactor and finishing flash. This eliminates the need for a final flash tank in the continuous process. Additionally, all storage tanks were designed to withstand upstream pressures. Furthermore, the continuous process has been modeled with newer design principles that in comparison to older methods of nylon-6,6 production require far less equipment[10]. Finally, to ensure proper solubility of the reactants the group is aware that the ADA solution needs to be at 212°F, this means that a heater is required for this reactant solution. In order to minimize the amount of equipment the group has designed the nylon-6,6 salt solution tank that is continuously stirred and heated to the necessary solubility temperature, this eliminates the need for multiple heat exchangers upstream of the solution tank.

Environmental

Nitrous oxide is not only hazardous, but also proves to have adverse effects on the atmosphere. In fact, 1 ton of nitrous oxide has “the equivalent climate change effect as 310 tons of CO_2”[27]. Nitrous oxide is a powerful greenhouse gas that contributes to global warming. Greenhouse gases accelerate global warming because they create a blanket-like effect on the Earth. The Environmental Protection Agency (EPA) has limited emissions of nitrous oxide, or a NOx gas. For Kentucky, the EPA has an emission limit for NOx gases of 40 tons/year[69]. There is an exception to this limit if the county in question has better than standard emission history for NOx gases. When researching Marshall County, the county where Calvert City is located, it was denoted that there was no data or that the county had better than standard emission rates[69]. This was not conclusive enough for the group to rule that we were under the emission limit and we included the capital cost and operating cost for a nitrous oxide scrubber for the nylon-6,6 process to reduce NOx emissions.

In addition to nitrous oxide's greenhouse gas effect, it is also able to react with the compounds in the atmosphere, which will destroy ozone. Nitrous oxide reacts in the stratosphere, the portion of the atmosphere that contains the protective ozone layer, and the reaction leads to ozone depletion[53]. Ozone (O_3) is a chemical compound that is a high oxidizer, but more than that, ozone provides a protective layer in the Earth's atmosphere. The ozone layer contains a higher concentration of ozone that absorbs ultra-violet (UV) radiation to prevent it from reaching the Earth's surface[53]. UV radiation has been linked to cancer, mostly skin cancers, and it is imperative for the Ozone layer to be able to absorb as much of the UV radiation as it can[19]. Nitrous oxide's effect on ozone had previously been overlooked, as it is a naturally occurring compound[37]. Nitrous oxide is naturally produced when bacteria consumes the nitrogen in soil or water[37]. Before the late 1990's, chlorofluorocarbons (CFCs) were the main concern of ozone depletion[25]. However, once the use of CFCs were phased out of use in the late 1990's, the emissions of nitrous oxide proved to be more concerning. The EPA and the states now regulate nitrous oxide emissions. The group has done research to understand the state of Kentucky's regulations and ensure that the nylon-6,6 process that has been designed will not violate any emission regulations.

As mentioned above, nitrous oxide is potentially introduced into the system via the ADA that is purchased from manufacturers. In most manufacturing processes of ADA where nitrous oxide is produced, the resulting product streams are then scrubbed to reduce the nitrous oxide emissions[39]. Most systems employ either thermal reduction of extended absorption and can achieve percentage reductions of nitrous oxide of up to 86%[39]. This however, is not 100% reduction of nitrous oxide and therefore the group has assumed that there will be nitrous oxide within the process.

Preliminary Hazard Analysis

Due to the limited amount of detailed information of the process that is available in the preliminary phases of design the group is only able to produce a preliminary hazard analysis. A detailed HAZOP will be required for the detailed design phase of this project. The format of the analysis is broken into three sections: overlap, batch, and continuous. The structure of the analysis follows the process-flow diagrams provided earlier in this document, Figures 1 and 2. The numbers listed refer to areas associated with the stream numbers in those diagrams. There was additional analysis conducted on each reactor due to the large number of hazards present in those pieces of equipment.

Overlap

1. HMDA Storage – The aqueous solution of HMDA is extremely corrosive[67]. This can lead to containment issues and the release of volatile, flammable vapors. This aqueous solution also is highly reactive with a large number of metals, and can be absorbed through skin. This risk can be mitigated by selecting storage vessels with adequate linings to ensure the wall of the storage tank is not compromised.

2. ADA Storage – ADA can create an explosive dust cloud if allowed to escape into the atmosphere. Additionally, it is recommended to store this chemical at temperatures below 77°F[2]. This risk can be mitigated by using an enclosed conveyor system for transporting the solid ADA and implementing a refrigeration system on the storage tank.

3. Water Storage – With the current information available the group found no apparent risks that could be mitigated, this should be re-evaluated during detailed design.

4. Salt Mixing Tank/Storage Tank – With the mixing and heating of the salt solution there is energy being added to the system, and there is also heat of mixing. With this energy addition that is concern of combustion. This risk can be mitigated with diluting the solution with large amounts of water and ensuring minimal to no contact with air. The preliminary design proposed includes the addition of large amounts of water for this purpose.

5. Centrifugal Pump – The mixed solution in the line is chemically stable, this is due to the mixing of an acid and base which results in a less volatile solution. There are two concerns with this area: cavitation, and solid ADA particulates in the line which will wear the pump blades. This risk can be mitigated by selected stronger metallurgy for the blades, and in the design proposed stainless steel was selected due to its strength in comparison to other options.

6. Pre-Feed Heat Exchanger – The concern with this area of the process is two phase flow downstream of the heater, before the reactor. This risk can be mitigated by implementing the control system proposed which includes a control valve prior to the reactor that is controlled by a level controller on the salt storage tank.

Batch

Reactor – Due to the high temperature within this reactor there is personnel risk if they are too close to the reactor. Additionally, there is a liquid and vapor stream exiting the reactor, this is phase separation. This leads to risks of shockwaves rattling the vessel. This risk can be mitigated by constructing additional structural support for the batch reactor, to ensure proper stability of the equipment. This should be further explored in detailed design.

7. Vapor Outlet of Reactor – There is a large volumetric of vapor traveling through this line. A major concern is containment issues and the fact that this stream holds nitrous oxide. This risk can be mitigated by implementing thick-walled piping to reduce loss of containment chances.

8. Liquid Outlet of Reactor – This stream is flowing at temperatures well above 500°F. This leads to large amounts of personnel risk. This risk can be mitigated by installing proper insulation on the lines transporting this stream.

9. Liquid stream of Flash Tank – There is a high temperature concern that is also present in 8. Additionally, with flash separation there is a large amount of noise generated which can damage personnel's' hearing. This risk can be mitigated by requiring double-hearing protection within a designated radius around the equipment.

10. Vapor stream of Flash Tank – Same concerns as number 7.

11. Positive Displacement Pump – This piece of equipment is transporting molten nylon-6,6. There is a concern of the molten polymer solidifying if there is a significant decrease in the line temperature. Furthermore, positive displacement pumps typically fail more often than centrifugal. This risk can be mitigated by purchasing the several spares that are costed in this preliminary design.

12. Extruder – Extrusion is the process of pushing a molten liquid through a die plate and allowing it to solidify and then slicing the extruded polymer into pellets. This process can lead to dramatic increases in pressure, and if the die plates becomes plugged dangerous pressure levels can be achieved. This risk can be mitigated by installing the emergency nylon-6,6 storage tank, and pressure control system that is proposed in this preliminary design.

13. Pellet Screen – The screening process is quite straightforward, and the main concern that was found is blockages. This risk can be mitigated by installing multiple screens and diverting product streams if there is a blockage in one screen. This should be explored further in detailed design.

Continuous

<u>PFR</u> – This reactor carries out the salt-formation reaction of the production of nylon-6,6. The salt will precipitate out and could plug the reactor. Additionally, this type of reactor can prove hard to monitor. This risk can be mitigated by implementing detailed control systems within the reactor, and should be explored in detailed design.

7. PFR Outlet Stream – Same as number 8 in the batch analysis.

8. Liquid stream of Flash Tank – Same as number 9 in the batch analysis.

9. Vapor stream of Flash Tank – Same as number 10 in the batch analysis.

<u>CSTR</u> – The condensation reaction that takes place in this reactor leads to a high density polymer. This leads to high amounts of strain on the mixer within this reactor. Additionally, there are vapor and liquid outlets in this reactor. This leads to the same risk mitigations presented in the batch reactor described earlier.

10. Vapor Outlet of Reactor – Same as number 7 in the batch analysis.

11. Liquid Outlet of Reactor – Same as number 8 in the batch analysis.

12. Positive Displacement Pump – Same as number 11 in the batch analysis.

13. Extruder – Same as number 12 in the batch analysis.

14. Pellet Screen – Same as number 13 in the batch analysis.

Other Important Considerations

The startup of the nylon-6,6 manufacturing plant was chosen as halfway through year two. This allows for ninety percent of the capital cost to be incurred and gives ample time for the construction phase to be completed. If this estimate proves too aggressive, startup times at the beginning of year three and the beginning of year four were evaluated in Tables A19 and A27 of the Appendix.

To appeal to a broad market, the group elected to pelletize the nylon product rather than spin it into strands. Additionally, there were no costing correlations found for the equipment in fiber spinning. A larger number of assumptions would have to be made in order to cost a spinning process than for the pelletizing process; this makes the economic analysis for a spinning process unfounded and uninformative. Furthermore, several companies that will purchase the nylon-6,6 product will melt it down before utilizing it in their manufacturing process[27]. Thus, extruding and granulating the final product is a more cost effective and time efficient option.

The chemical price industry can experience volatility over time, so the prices of the nylon-6,6 product and the reactants are subject to change. This variability in the sales price as well as the raw material costs are discussed in the Economic Analysis section under sensitivity analysis. Further detail can be found in the sensitivity analysis section of the Appendix.

EPA standards limit the amount of NO_x from combustion of high nitrogen content fuels[39]. In the furnaces used for heating both process designs, methane is used as the fuel gas. Methane is a relatively low nitrogen fuel, but the content of nitrogen in the fuels should be considered when flaring the excess gas to the atmosphere.

Manufacturing Costs

The cost of manufacturing was estimated using Equation (36) shown below.

$$COM = 0.280FCI + 2.73C_{OL} + 1.23(C_{UT} + C_{WT} + C_{RM}) \tag{36}$$

Fixed Capital Investment, FCI

The fixed capital investment is the total grass roots cost. This was calculated as shown in the Fixed Capital Investment Summary section.

Operating Labor Costs, C_{OL}

The operating labor costs were estimated using Equations (37) to (41). The hourly wage of workers was calculated with Equation (40) using the minimum wage in Kentucky[12]. The factor of 1.5 to determine the hourly operator wage was selected as it resulted in a yearly wage comparable to operator yearly salaries[68].

$$N_{OL} = \sqrt{6.29 + +31.7P^2 + 0.23N_{np}} \tag{37}$$

$$N_{np} = \Sigma Equipment \tag{38}$$

$$RN_{OL} = 4.5N_{OL} \tag{39}$$

$$W_O = 1.5 * W_{min} \tag{40}$$

$$C_{OL} = RN_{OL}W_oH_{op} \tag{41}$$

Utility Costs, C_{UT}

The utility costs were calculated based on the rates as shown in Table 37 below.

Table 37. Utility Rates

Utility	Cost/unit
Power [21][63]	$0.06746/kWh and correlation
Fuel Gas [39][62]	$11.1/GJ and correlation
High pressure steam (sat) [62]	$29.97/1000 kg
Med pressure steam (sat) [62]	$29.95/1000 kg
Low pressure steam (sat) [62]	$29.29/1000 kg
Paratherm HT [46]	Hot oil correlation
Cooling water [62]	$14.8/1000m3

The hot oil correlation used is as shown in Equations (42) to (43)[64].

$$U_{oil} = (6.0 * \ 10^{-7}) Q_H (T^{0.5}) \tag{42}$$

$$C_{oil} = \ U_{oil} Q_H \tag{43}$$

Additional power costs were incurred for the extruder. Based on the capacity provided by the manufacturer, 5 extruders were required[63]. The power cost for extruders was calculated utilizing the rate that an extruder consumes 120 kW[63].

Additional utility costs were incurred for the fuel gas burning nitrous oxide in the scrubber. These costs were calculated based on a rate from the EPA that says the scrubber material cost is $650/ton of nitrous oxide passing through the scrubber[39].

Waste Treatment Costs, C_{WT}

The waste treatment cost was estimated using the heuristic that wastewater treatment costs $41/1000m^3[62]. The flow stream leaving the nitrous oxide scrubber was treated.

Raw Material Costs, C_{RM}

The raw material costs were calculated based on the rates shown in Table 38 below.

Table 38. Raw Material Prices

Material	Price (USD)
Adipic Acid [27]	$1.50/kg
HMDA [27]	$2.50/kg
Deionized Water [62]	$1/1000kg

Hours of Operation

All of the raw material, utility, and waste flow rates used in the calculations relied on the number of operating hours in one year. A service factor of 0.96 was used for yearly operation calculations[62].

$$D_{op} = 0.96 * 365 \tag{44}$$

The number of operating hours per year was then calculated separately for the batch and continuous options.

For the batch process, the batch feed time was optimized to be two hours. The down time was calculated by first calculating the time it would take to drain the batch reactor utilizing Equation (45)[62]. A 2-inch schedule-40 pipe was assumed to be the exit piping of the batch process[62].

$$H_{fill} = \frac{4(0.6V_{batch})}{\pi D_{batch}} \tag{45}$$

$$\frac{dH}{dt} = \frac{-\sqrt{2g}A_p}{A_t}\sqrt{H} \tag{46}$$

Evaluating the derivative shown in Equation (46) from H_{fill} to 0 resulted in a draining time of 20 minutes. It was then assumed that three times this value, 60 minutes, would be a reasonable estimate for the downtime. Using the batch feed time of two hours and down time of 1 hour, the operating hours per year of the batch process was calculated with Equations (47) to (48).

$$t_{batch} = \frac{24}{t_{down} + t_{feed}} * \ t_{feed} \tag{47}$$

$$H_{op,batch} = t_{batch}D_{op} \tag{48}$$

For the continuous process, the days operating is equal to D_{op}. Therefore, to calculating the hours operating per year was simply a unit conversion shown in Equation (49).

$$H_{op,cont} = \ D_{op} * 24 \tag{49}$$

Using these operational hours for each process, the yearly flowrates of raw materials, utilities, and waste were calculated and the cost of manufacturing was determined.

Manufacturing Costs Summary

The key costs calculated for each process are shown below in Table 39.

Table 39. Summary of Costs for Design Process

Key Cost	Batch	Continuous
Fixed Capital Investment	$21,000,000	$16,000,000
Raw Material Cost	$59,000,000	$88,000,000
Waste Treatment Cost	$ 2,020	$3,100
Utility Cost	$ 4,500,000	$1,500,000
Operating Labor Cost	$ 3,200,000	$4,900,000
Number of Equipment	5	7
Compressors	0	0
Towers	1	1
Reactors	1	2
Heaters	1	2
Exchangers	2	2
Cost of Manufacturing	$92,000,000	$130,000,000

Economic Analysis

Cost of Manufacturing

The cost of manufacturing of each process was used as the annual operating cost. The table above in the Manufacturing Costs section outlines the breakdown of the operating cost for raw materials, utilities, waste treatment, and operating labor. The cost of manufacturing was calculated using the equations discussed in the Manufacturing Costs section from the Turton textbook[62]. Total costs of manufacturing for both the batch process and the continuous process are shown in Table 40 below.

Table 40. Cost of Manufacturing for Design Processes

	COM
Batch Process	$ 92,000,000
Continuous Process	$ 128,000,000

The cost of manufacturing for the continuous process is greater than that for the batch process because of the hours of operation. The continuous process has a service factor of 0.96, or it operates for 8410 hours per year. The batch process has a significant amount of downtime associated with its operation, and it only operates for 5606 hours per year. This difference in annual operating times accounts for most of the manufacturing cost increase from the batch process to the continuous process design.

Investment Strategy

Capital costs in the construction process were assumed to be divided over three years, with the majority of the cost incurred in the initial year. The breakdown of capital costs by year is shown in Table 41.

Table 41. Investment Strategy for Capital Costs

Year	Capital Cost Incurred
0	60%
1	30%
2	10%

Startup of production was assumed to begin halfway through year two, and then full-scale production would begin the following year. In the sensitivity analyses that are discussed later in this section, this startup time was adjusted to the beginning of year three and the beginning of year four to determine its effect on the overall project economics.

Reactor Economic Optimization

The processes were first optimized for the technical requirements. Process temperatures, pressures, and flow rates were adjusted and process equipment was given initial specifications as a starting point for the economic optimization and evaluation. The technical optimization is discussed is the Process Description section of the report.

To appropriately cost the reactors in each of the two processes, they were treated as a vessel and heat exchanger[66]. This was introduced above in the equipment costing sections. Given a required volume of a reactor from the technical optimization, the length to diameter ratio of the vessel portion was varied to minimize the cost of the reactor. For economic optimization, the volume and L/D ratio was varied and the impact on the cost of the vessel for the reactor was analyzed. Only the impact on the vessel cost was investigated as a change in volume and L/D primarily affect the vessel.

For the batch process, one reactor was used. The required volume for the batch process was 46.7 cubic meters. The L/D ratio was varied and the trends observed. As the L/D ratio decreases, the capital cost for the vessel used as the reactor increases. This is demonstrated in Table 42 below. Despite the cheapest option as the highest length to diameter ratio, the group limited the L/D to a maximum of three due to concerns of incomplete mixing at higher ratios[62]. The bold row in the table indicates the selection for the best batch vessel configuration.

Table 42. Batch Reactor Dimensions Optimization

Volume (m^3)	46.7	***Vertical Vessel**		
Maximum Pressure (barg)	4.05			
L/D	**Height**	**Diameter**	**MOC**	**GR Costs**
3.38	8.80	2.6	SS	$ 780,000
3.02	**8.16**	**2.7**	**SS**	**$ 790,000**
2.71	7.58	2.8	SS	$ 810,000
2.44	7.07	2.9	SS	$ 820,000

The group also investigated a process using two batch reactors in parallel. This would reduce the material flow through each reactor and cut the necessary volume in half. The length to diameter ratios were varied at similar values. This is summarized below in Table 43. Dividing the flow into two parallel streams is not economically attractive because the capital cost for two batch reactors is significantly larger than that for one reactor with a bigger volume.

Table 43. Parallel Batch Reactors Dimension Optimization

Volume (m^3)	23.35	***2 Vertical Vessels in Parallel**			
Maximum Pressure (barg)	4.05				
L/D	**Height**	**Diameter**	**MOC**	**GR Costs / Unit**	**GR Costs**
3.72	7.43	2	SS	$ 400,000	$ 800,000
2.99	6.43	2.15	SS	$ 410,000	$ 830,000
2.44	5.62	2.3	SS	$ 430,000	$ 860,000

The same process was used for the plug flow reactor and the CSTR in the continuous process. Heuristics for PFRs indicate that the appropriate length to diameter ratio is above 25[65]. Given an initial volume of 120.1 cubic meters, the L/D ratio was varied from about 25 to 90. Table 44 below shows the results from this analysis. The best length to diameter ratio was determined to be approximately 38. The bold row in the table below indicates the best PFR dimensions for a volume of 120.1 cubic meters.

Table 44. PFR Dimension Optimization: Initial Volume

Volume (m^3)	120.1	***Horizontal Vessels in Series**		
Maximum Pressure (barg)	4.05			
L/D	**Length**	**Diameter**	**MOC**	**GR Costs**
26.22	47.20	1.8	SS	$ 960,000
31.12	52.91	1.7	SS	$ 940,000
34.04	56.17	1.65	SS	$ 930,000
37.33	59.73	1.6	SS	$ 920,000
38.04	**60.49**	**1.59**	**SS**	**$ 910,000**
41.06	63.65	1.55	SS	$ 1,030,000
45.31	67.96	1.5	SS	$ 1,010,000

55.73	78.02	1.4	SS	$ 1,060,000
69.60	90.48	1.3	SS	$ 1,060,000
88.49	106.2	1.2	SS	$ 1,120,000

The volume of the PFR affects the conversion of the reaction. The group investigated increasing or decreasing the volume of the PFR and its effects on the amount of nylon-6,6 generated in the reaction and the capital cost of the reaction vessel. First, the PFR vessel increased to 190.7 cubic meters. The results from the L/D optimization are shown in Table 45 below.

Table 45. PFR Dimension Optimization: Large Volume

Volume (m^3)	190.7	***Horizontal Vessels in Series**		
Maximum Pressure (barg)	4.05			
L/D	**Length**	**Diameter**	**MOC**	**GR Costs**
25.40	53.34	2.1	SS	$ 1,400,000
30.35	60.70	2	SS	$ 1,400,000
35.40	67.26	1.9	SS	$ 1,380,000
37.73	70.19	1.86	SS	$ 1,360,000
38.35	70.95	1.85	SS	$ 1,360,000
41.64	74.94	1.8	SS	$ 1,500,000

The change in the size of the reactor did not have a significant effect on the conversion achieved. Nearly all of the reactants had been converted to nylon-6,6 in the 120.1 cubic meter reactor, so the increase in size does not increase the return. Because of the larger volume, the capital cost is greater, so increasing the reactor size is not economically attractive. Compared to the slight increase this would cause in raw material cost.

If the volume of the PFR is decreased to 35.6 cubic meters, the reaction still nearly proceeds to completion. A smaller reactor will have a lower capital cost, but return nearly the same conversion. Thus, decreasing the reactor size is the best option. The length to diameter ratio was varied in the same manner as it was with the other two sizes. Again, the optimal L/D value was found to be approximately 38. The results from this analysis are show in Table 46 below, with the bolded row indicating the selection for the PFR vessel.

Table 46. PFR Dimension Optimization: Small Volume

Volume (m^3)	35.6	***Horizontal Vessels in Series**		
Maximum Pressure (barg)	4.05			
L/D	**Length**	**Diameter**	**MOC**	**GR Costs**
20.62	26.81	1.3	SS	$ 380,000
26.22	31.46	1.2	SS	$ 370,000
29.79	34.26	1.15	SS	$ 370,000
34.04	37.44	1.1	SS	$ 360,000

38.04	**40.32**	**1.06**	**SS**	**$**	**360,000**
39.14	41.09	1.05	SS	$	360,000
45.31	45.31	1	SS	$	420,000
62.15	55.93	0.9	SS	$	480,000

Figure 9 below clearly shows the smallest diameter reactor to be the best economic investment given that all three produce nearly the same conversion and outflow of nylon-6,6.

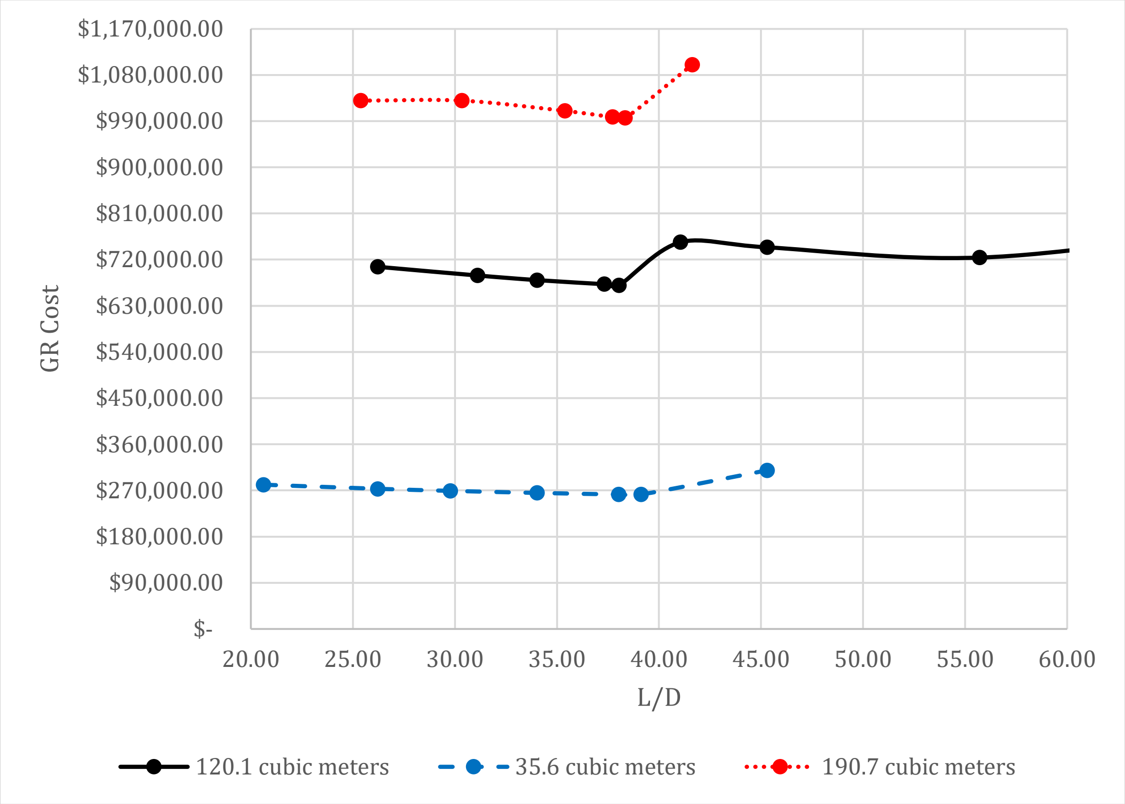


Figure 9. PFR Dimension Optimization Summary

The apparent discontinuities in the graph are caused by the costing method used. The reactor vessel was treated as several vessels in series due to the large length to diameter ratio. The jumps in each series represent a critical L/D where a new vessel in series is needed to meet the length.

The CSTR length to diameter ratio was set to a value of one based on a heuristic for polymer systems[65]. Despite this, the group still investigated the effect L/D ratio on the CSTR vessel cost. The dimensions of the CSTR vessel did not influence the capital cost to any significant degree, so the heuristic value was used. Table 47 below summarizes these results.

Table 47. CSTR Dimension Optimization

Volume (m^3)	1.812	***Vertical Vessel**		
Maximum Pressure (barg)	1.013			
L/D	**Length**	**Diameter**	**MOC**	**GR Costs**
3.16	2.85	0.9	SS	$ 65,000
2.96	2.73	0.92	SS	$ 65,000
2.31	2.31	1	SS	$ 65,000
1.73	1.91	1.1	SS	$ 65,000
1.34	1.60	1.2	SS	$ 65,000
1.05	1.37	1.3	SS	$ 65,000
1.00	**1.32**	**1.32**	**SS**	**$ 65,000**

Revenue

The costs of ADA and HMDA were taken from the Invista Corporation as 1500 and 2500 USD per metric ton, respectively[27]. These values were checked using data taken from the UN Comtrade statistics for imports and exports involving the United States. Sales prices for small quantities within the UN Comtrade database of either reactant were ignored due to the misrepresentation of the cost of transportation of the chemical versus the material cost. These values corroborated the given prices; they were within ten percent price variation per kilogram.

The sales price for nylon-6,6 pellets were then estimated using the same statistics database[61]. Treating small quantity sales as outliers and taking the median value from the remaining data, the sales price of nylon-6,6 pellets was estimated at 5.06 USD per kilogram, or 2.29 USD per pound. The ratio of the nylon-6,6 sales price to the ADA and HMDA purchase prices was also validated using standard chemical suppliers[7][8].

Batch Design Economic Evaluation

Using a ten year project life and ten year MACRS depreciation values, a cash flow table for the batch process design was generated. Because the plant will be a grass roots facility, the corporate financial situation was assumed to be stand alone. In years where the process is not profitable, the company does not get a tax break, but rather, uses the previous year's expense as a loss forward entry in the next year. The corporate tax rate for the cash flow analysis was assumed to be forty percent. With a set hurdle rate of fifteen percent, the batch design has a net present value of 73.3 million USD. The cash flow table is shown in the following page.

Table 48. Batch Process Cash Flow

Project Title: **Batch Design**
Corporate Financial Situation: *Stand Alone*
Minimum Rate of Return: 0.15 or 15.0%
1 = $1.00 ** Startup halfway through year 2
Equipment Cost $20,893,410.91

End of Year	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Production (lb/hr)	0	0	10,214	10,214	10,214	10,214	10,214	10,214	10,214	10,214	10,214
Hours of operation (hr/yr)	0	0	2,803	5,606	5,606	5,606	5,606	5,606	5,606	5,606	5,606
x Sales Price ($/lb)	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29
Sales Revenue	0	0	65,664,732	131,329,463	131,329,463	131,329,463	131,329,463	131,329,463	131,329,463	131,329,463	131,329,463
+ Salvage Value											
- Royalties											
Net Revenue	0	0	65,664,732	131,329,463	131,329,463	131,329,463	131,329,463	131,329,463	131,329,463	131,329,463	131,329,463
- ADA Material Cost			(12,518,831)	(25,037,662)	(25,037,662)	(25,037,662)	(25,037,662)	(25,037,662)	(25,037,662)	(25,037,662)	(25,037,662)
- HMDA Material Cost			(16,729,386)	(33,458,772)	(33,458,772)	(33,458,772)	(33,458,772)	(33,458,772)	(33,458,772)	(33,458,772)	(33,458,772)
- Deionized Water Material Cost			(22,549)	(45,098)	(45,098)	(45,098)	(45,098)	(45,098)	(45,098)	(45,098)	(45,098)
- Cooling Water Operating Cost			0	0	0	0	0	0	0	0	0
- Fuel Gas Operating Cost			(2,003,284)	(4,006,568)	(4,006,568)	(4,006,568)	(4,006,568)	(4,006,568)	(4,006,568)	(4,006,568)	(4,006,568)
- Paratherm Operating Costs			(580)	(1,159)	(1,159)	(1,159)	(1,159)	(1,159)	(1,159)	(1,159)	(1,159)
- LPS Operating Costs			(113,267)	(226,534)	(226,534)	(226,534)	(226,534)	(226,534)	(226,534)	(226,534)	(226,534)
- Electricity Operating Costs			(114,080)	(228,160)	(228,160)	(228,160)	(228,160)	(228,160)	(228,160)	(228,160)	(228,160)
- Other Operating Costs			(14,591,317)	(29,182,634)	(29,182,634)	(29,182,634)	(29,182,634)	(29,182,634)	(29,182,634)	(29,182,634)	(29,182,634)
- Depreciation		(1,253,605)	(2,883,291)	(3,142,369)	(2,722,829)	(2,178,765)	(1,742,510)	(1,475,702)	(1,385,651)	(1,369,772)	(1,369,145)
- Loss Forward			(1,253,605)								
- Writeoffs											(1,369,772)
Taxable Income	0	(1,253,605)	15,434,542	36,000,506	36,420,046	36,964,110	37,400,365	37,667,174	37,757,224	37,773,103	36,403,958
-Tax @ 40%	0	0	(6,173,817)	(14,400,202)	(14,568,018)	(14,785,644)	(14,960,146)	(15,066,869)	(15,102,890)	(15,109,241)	(14,561,583)
Net Income	0	(1,253,605)	9,260,725	21,600,304	21,852,028	22,178,466	22,440,219	22,600,304	22,654,334	22,663,862	21,842,375
+ Depreciation		1,253,605	2,883,291	3,142,369	2,722,829	2,178,765	1,742,510	1,475,702	1,385,651	1,369,772	1,369,145
+ Loss Forward		0	1,253,605	0	0	0	0	0	0	0	0
+ Writeoffs		0	0	0	0	0	0	0	0	0	1,369,772
- Working Capital											
- Fixed Capital	(12,536,047)	(6,268,023)	(2,089,341)								
Cash Flow	(12,536,047)	(6,268,023)	11,308,280	24,742,673	24,574,857	24,357,231	24,182,729	24,076,006	24,039,985	24,033,634	24,581,292
Discount Factor ($P/F_{i,n}$)	1.0000	0.8696	0.7561	0.6575	0.5718	0.4972	0.4323	0.3759	0.3269	0.2843	0.2472
Discounted Cash Flow	(12,536,047)	(5,450,455)	8,550,684	16,268,709	14,050,754	12,109,849	10,454,861	9,051,062	7,858,714	6,831,859	6,076,119
Net Present Value	**73,266,110**										
DCFROR	**68.92%**										
Undiscounted Payback Period	**2.39**										

The group performed a sensitivity analysis on the above cash flow by varying parameters that would affect the net worth of the project. Table 49 below shows the parameters which were varied per heuristic values[62].

Table 49. Sensitivity Analysis Parameter Variation

Variable	Low Value	High Value
Sales Price of Nylon 6,6	- 20%	+ 20%
Purchase Price of ADA	- 20%	+ 20%
Purchase Price of HMDA	- 20%	+ 20%
Equipment Costs	- 25%	+ 40%
Operating Costs	- 25%	+ 40%
Project Life	7 years	15 years

The startup time for production in the plant was also varied with a base case of halfway through year 2. The other values investigated were a startup time at the beginning of year 3, and at the beginning of year 4.

The effect of each variable on the net present value was examined and a tornado chart was developed summarizing the results. The sales price of nylon-6,6 has the greatest effect of the NPV of the project followed by the operating costs and the project life. The equipment cost had the least effect on the NPV of the project.

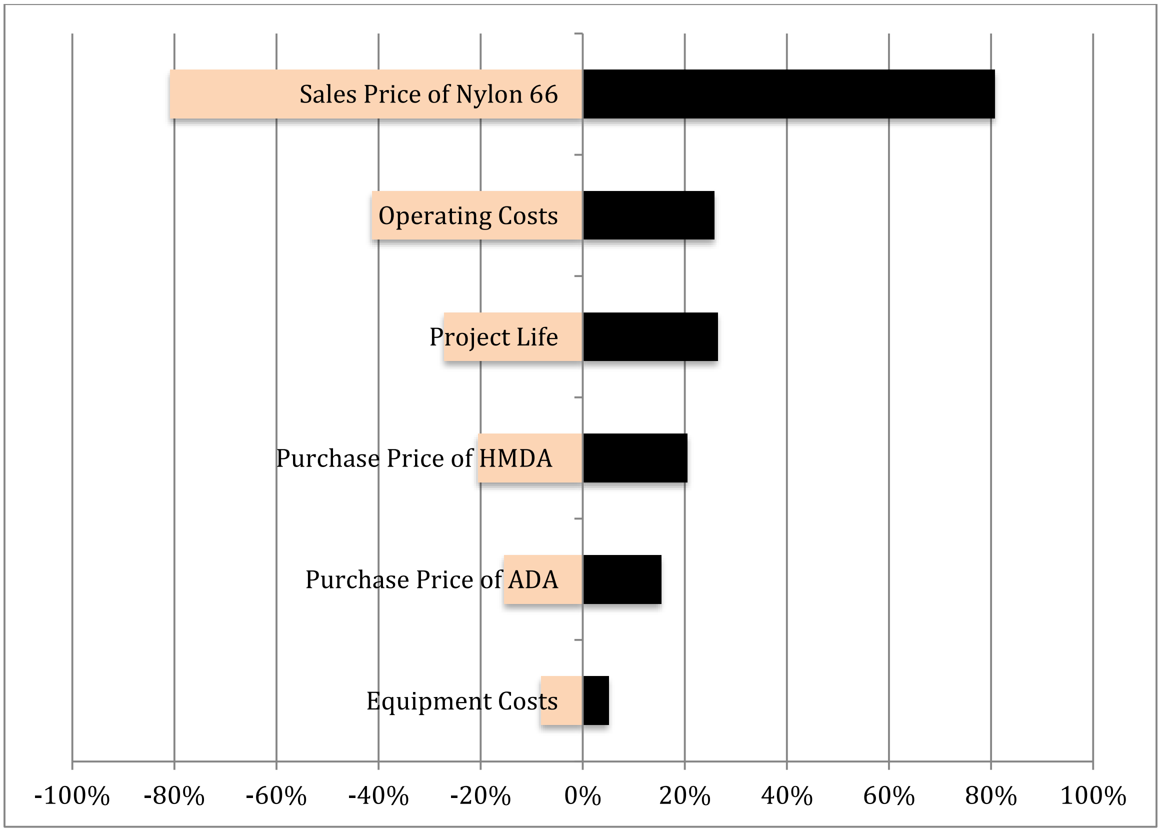


Figure 10. Tornado Chart for Batch Process Sensitivity Analysis

Tables and graphs for each varied parameter and their individual effect on the net present value of the project can be found in the Appendix of the report.

The range of values for the NPV produced from the sensitivity analyses are shown in a table below. The worst case scenario is determined using all of the undesirable variations in the parameters to get the lowest NPV that could be realized by the project. Similarly, the best case scenario is determined using all of the desirable variations in the parameters considered.

Table 50. Overall Range of Batch Sensitivity Analysis

Batch Design	Base Case	Worst Scenario	Best Scenario
NPV (USD)	73,300,000	(50,300,000)	225,000,000

Continuous Design Economic Evaluation

A cash flow table for the continuous process was generated using the same specifications as the batch design. The cash flow assumed a ten year project life and utilized ten year MACRS depreciation, which is standard for industrial equipment. The corporate financial situation was stand alone and the tax rate was set at forty percent. Using a hurdle rate of fifteen percent, the net present value of the project was determined to be 144 million USD. The cash flow table is shown in the following page.

Table 51. *Continuous Process Cash Flow*

Project Title:		**Continuous Design**	
Corporate Financial Situation:		*Stand Alone*	
Minimum Rate of Return:	0.15	or	15.0%
1 = $1.00		** Startup halfway through year 2	

Equipment Cost $16,005,691.36

End of Year	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Production (lb/hr)	0	0	10,214	10,214	10,214	10,214	10,214	10,214	10,214	10,214	10,214
Hours of operation (hr/yr)	0	0	4,205	8,410	8,410	8,410	8,410	8,410	8,410	8,410	8,410
x Sales Price ($/lb)	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29	$2.29
Sales Revenue	0	0	98,497,097	196,994,195	196,994,195	196,994,195	196,994,195	196,994,195	196,994,195	196,994,195	196,994,195
+ Salvage Value											
- Royalties											
Net Revenue	0	0	98,497,097	196,994,195	196,994,195	196,994,195	196,994,195	196,994,195	196,994,195	196,994,195	196,994,195
- ADA Material Cost			(18,908,274)	(37,816,549)	(37,816,549)	(37,816,549)	(37,816,549)	(37,816,549)	(37,816,549)	(37,816,549)	(37,816,549)
- HMDA Material Cost			(25,267,783)	(50,535,566)	(50,535,566)	(50,535,566)	(50,535,566)	(50,535,566)	(50,535,566)	(50,535,566)	(50,535,566)
- Deionized Water Material Cost			(34,058)	(68,115)	(68,115)	(68,115)	(68,115)	(68,115)	(68,115)	(68,115)	(68,115)
- Cooling Water Operating Cost			0	0	0	0	0	0	0	0	0
- Fuel Gas Operating Cost			(363,892)	(727,783)	(727,783)	(727,783)	(727,783)	(727,783)	(727,783)	(727,783)	(727,783)
- Paratherm Operating Costs			(1,041)	(2,082)	(2,082)	(2,082)	(2,082)	(2,082)	(2,082)	(2,082)	(2,082)
- LPS Operating Costs			(184,523)	(369,047)	(369,047)	(369,047)	(369,047)	(369,047)	(369,047)	(369,047)	(369,047)
- Electricity Operating Costs			(171,928)	(343,855)	(343,855)	(343,855)	(343,855)	(343,855)	(343,855)	(343,855)	(343,855)
- Other Operating Costs			(19,206,172)	(38,412,344)	(38,412,344)	(38,412,344)	(38,412,344)	(38,412,344)	(38,412,344)	(38,412,344)	(38,412,344)
- Depreciation		(960,341)	(2,208,785)	(2,407,256)	(2,085,862)	(1,669,073)	(1,334,875)	(1,130,482)	(1,061,497)	(1,049,333)	(1,048,853)
- Loss Forward			(960,341)								
- Writeoffs											(1,049,333)
Taxable Income	0	(960,341)	31,190,300	66,311,597	66,632,991	67,049,779	67,383,978	67,588,371	67,657,355	67,669,520	66,620,667
-Tax @ 40%	0	0	(12,476,120)	(26,524,639)	(26,653,196)	(26,819,912)	(26,953,591)	(27,035,348)	(27,062,942)	(27,067,808)	(26,648,267)
Net Income	0	(960,341)	18,714,180	39,786,958	39,979,795	40,229,868	40,430,387	40,553,023	40,594,413	40,601,712	39,972,400
+ Depreciation		960,341	2,208,785	2,407,256	2,085,862	1,669,073	1,334,875	1,130,482	1,061,497	1,049,333	1,048,853
+ Loss Forward		0	960,341	0	0	0	0	0	0	0	0
+ Writeoffs		0	0	0	0	0	0	0	0	0	1,049,333
- Working Capital											
- Fixed Capital	(9,603,415)	(4,801,707)	(1,600,569)								
Cash Flow	(9,603,415)	(4,801,707)	20,282,737	42,194,214	42,065,656	41,898,941	41,765,262	41,683,505	41,655,911	41,651,045	42,070,586
Discount Factor ($P/F_{i,n}$)	1.0000	0.8696	0.7561	0.6575	0.5718	0.4972	0.4323	0.3759	0.3269	0.2843	0.2472
Discounted Cash Flow	(9,603,415)	(4,175,398)	15,336,663	27,743,381	24,051,176	20,831,179	18,056,275	15,670,373	13,617,391	11,839,827	10,399,205
Net Present Value	**143,766,657**										
DCFROR	**117.70%**										
Undiscounted Payback Period	**1.79**										

A similar sensitivity analysis was performed for the continuous process design, with the parameters varying by the same factors. A tornado chart of the effect of the parameter variation on the NPV is presented below.

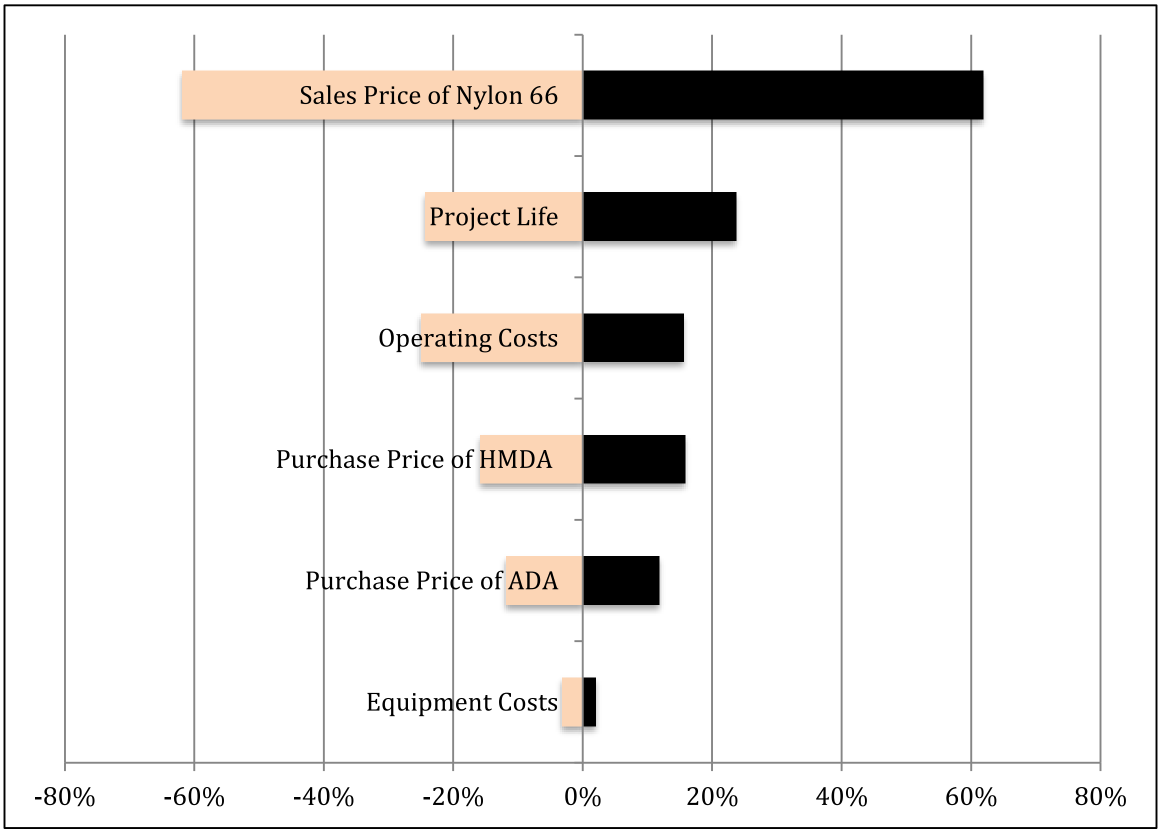


Figure 11. Tornado Chart for Continuous Sensitivity Analysis

Tables and graphs for each varied parameter and its effect on the net present value can be found in the Appendix of the report.

Using the same method as before, a range of values for the NPV of the project was developed using the undesirable parameter variations and the desirable parameter variations. The results from this analysis are presented below in Table 52.

Table 52. Overall Range of Continuous Sensitivity Analysis

Overall Range of Sensitivity Analysis			
Continuous Design	**Base Case**	**Worst Scenario**	**Best Scenario**
NPV (USD)	144,000,000	(28,900,000)	366,000,000

Incremental Analysis

An incremental analysis was performed on the two projects to determine the more economically attractive option. Using the discounted cash flows of each project and subtracting the annual batch cash flow from the continuous cash flow, the continuous project was determined to be the best economic option. The net present value of the incremental analysis is 70.5 million dollars in favor of the continuous process. The incremental analysis does not show any negative cash flows because the capital costs of the continuous design are lower, but the revenues are larger. Table 53 outlining the incremental analysis is shown below.

Table 53. Incremental Analysis

Discounted Cash Flow			
Year	**Batch (A)**	**Continuous (B)**	**Incremental (B-A)**
0	$(12,500,000)	$(9,600,000)	$2,900,000
1	$(5,500,000)	$(4,200,000)	$1,300,000
2	$8,600,000	$15,300,000	$6,800,000
3	$16,300,000	$27,700,000	$11,500,000
4	$14,100,000	$24,100,000	$10,000,000
5	$12,100,000	$20,800,000	$8,700,000
6	$10,500,000	$18,100,000	$7,600,000
7	$9,100,000	$15,700,000	$6,600,000
8	$7,900,000	$13,600,000	$5,800,000
9	$6,800,000	$11,800,000	$5,000,000
10	$6,100,000	$10,400,000	$4,300,000
Total NPV	$73,300,000	$143,800,000	**$70,500,000**

Refer to Table 54 for both process options below. The tables present the capital costs, present worth costs, net present values, rates of return, and the undiscounted payback periods for the batch process alongside the more economically attractive continuous design.

Table 54. Economic Summary

	Batch Process	**Continuous Process**
Net Present Value (USD)	$73,300,000	$144,000,000
DCFROR	68.9%	117.7%
Undiscounted Payback Period (yrs)	2.39	1.79
Capital Costs (USD)	$20,900,000	$16,000,000
Present Worth Cost (USD)	($226,000,000)	($304,000,000)

Conclusions and Recommendations

Conclusions

After evaluation of both the continuous and batch processes proposed, the group has selected to recommend the continuous process for detailed design. This selection was made in regards to the more appealing economics associated with the continuous design in comparison to the batch process. Additionally, after a preliminary hazard analysis it was determined that there was not a significant change in risk between the process options. Furthermore, the continuous process is utilized in several plants across the US[10][27]. The design proposed is validated by being modeled after several patented processes, and was modeled on Aspen Plus Polymers to ensure that the correct amount of nylon-6,6 could be produced[10].

The group also concludes that the continuous design is more than economically feasible to be constructed. This was determined by evaluating the NPV of the project and conducting a thorough sensitivity analysis. It is noted that there were some cases discovered during the sensitivity analysis where the continuous process was deemed not to be economically attractive. However, these cases were extreme and mainly dependent upon the sales price of nylon-6,6. Additionally, there are several economic forecasts that show the demand of nylon-6,6 on the rise and thus, it is unlikely that the price will decrease[42]. Below is a summary of the NPV of the two evaluated processes.

Table 55. NPV for Process Designs

Batch	Continuous
$73,300,000	$144,000,000

Along with this design is a proposed controls system. This system was implemented to mitigate the risk of several hazardous areas within the process. This control system elevates the inherent safety of the design, and allows a more streamlined process to be put into place. Additionally, it was noted that the group should propose a system that handles the side products from this process, the group addressed this concern with the addition of the nitrous oxide scrubber that is described in the equipment specifications section of this report[47]. Along with the other hazard analyses, the interactions of the raw materials were evaluated. Materials of construction were researched to ensure that the interactions between the raw materials and the materials of construction would not result in a catastrophic event.

Recommendations

A preliminary control system was designed as shown in the process flow diagrams for the two processes. This control system should be evaluated and expanded upon in detailed design.

Evaluation of the 67% turndown case includes examining pump curves to ensure that pumps can operate at reduced capacity, determining line sizing required to ensure that no two phase flow occurs with decreased flow rates, and re-evaluating utility flow rates. These calculations were determined to be out of the scope of this preliminary design. As a result, all of these factors involved with the 67% turndown case should be addressed in detailed design.

Storage tanks were costed without incorporating material of construction considerations. As a result, the costs of these tanks should be re-evaluated in detailed design with different cost correlations. The materials for the storage tanks are as follows.

Table 56. Materials of Construction for Storage Tanks

Storage Tank	Material of Construction
HMDA	Titanium Steel
ADA	Stainless Steel
Water	Carbon Steel
Nylon-6,6 Pellets	Carbon Steel

Additionally, the costs should be escalated to a more appropriate timeline once construction years have been selected. Costs are currently escalated to June 2016.

Certain equipment was too small to cost with the given correlations and was therefore costed at the minimum sizing parameter value. These pieces of equipment should be resized and the costs associated with them re-evaluated. For the batch process, these pieces of equipment include: salt mixer, pre-feed heat exchanger, HMDA pump, and deionized water pump. For the continuous process these pieces of equipment include: CSTR heat exchanger, CSTR furnace, CSTR mixer, salt mixer, pre-feed heat exchanger, HMDA pump, and deionized water pump.

Further investigation should be done in detailed design to understand the duty profile within the PFR and CSTR and the costs associated with the cooling required as the profiles provided in preliminary design showed no need for a cooling water system.

The preliminary hazard analysis will have to be expanded upon in detailed design to create a full HAZOP report for the process. Once the process is in place, any material in contact with the HMDA aqueous solution will require frequent checking as HMDA is highly corrosive to all metals[67].

Acknowledgments

The design group would like to acknowledge the American Institute of Chemical Engineers as the developers of this project. Additionally, we would like to give thanks to Invista Corporation for providing raw material costing information.

Bibliography

[1] *Adipic Acid, Compound with Hexane-1,6-diamine (1:1)*. Material Safety Data Sheet. Solvay, 2012.

[2] *Adipic Acid MSDS*. Material Safety Data Sheet. ScienceLab.com, 2013.

[3] Anderson, William C. *Innovative Site Remediation Technology: Chemical Treatment*. Washington, D.C.: U.S. Environmental Protection Agency, Solid Waste and Emergency Response, 1994. Print.

[4] Anderson, William C. *Innovative Site Remediation Technology: Solvent/Chemical Extraction*. Washington, D.C.: U.S. Environmental Protection Agency, Solid Waste and Emergency Response, 1995. Print.

[5] Aspen Technology, Inc. *Aspen Polymers: User Guide Volume 1*. Burlington, MA: Aspen Technology, 2011. Print.

[6] Aumi, Siam, Brandon Corbett, Prashant Mhaskar, and Tracy Clarke-Pringle. "Data-Based Modeling and Control of Nylon-6, 6 Batch Polymerization." *IEEE Transactions on Control Systems Technology* 21.1 (2013): 94-106. Web.

[7] "A13705 Adipic Acid, 99%." *124-04-9 - Adipic Acid, 99% - Butane-1,4-Dicarboxylic Acid - Hexanedioic Acid - A13705 - Alfa Aesar*, www.alfa.com/en/catalog/A13705/. Accessed 21 Feb. 2017.

[8] "A14212 1,6-Diaminohexane, 98+%." *124-09-4 - 1,6-Diaminohexane, 98+% - Hexamethylenediamine - 1,6-Hexanediamine - A14212 - Alfa Aesar*, www.alfa.com/en/catalog/A14212/. Accessed 21 Feb. 2017.

[9] Baukal, Charles and Bussman, Wes. "Simulator for Teaching Process Heater Operating Principles." *American Society for Engineering Education* (2009):. Web.

[10] Beaton, Daniel Harper. Continuous Solid-Phase Polymerization of Polyamide Granules. E.I. Du Pont De Nemours and Company, assignee. Patent 3821.171. 28 June 1974. Print.

[11] Beloff, Beth, Marianne Lines, and Dicksen Tanzil. *Transforming Sustainability Strategy into Action: The Chemical Industry*. Hoboken: Wiley-VCH, 2005. Print.

[12] Brainerd, Jackson. "State Minimum Wages | 2017 Minimum Wage by State." *State Minimum Wages | 2017 Minimum Wages by State*, www.ncsl.org/research/labor-and-employment/state-minimum-wage-chart.aspx. Accessed 1 Mar. 2017.

[13] CDC. *ADIPIC ACID*. CDC, 1 July 2014, https://www.cdc.gov/niosh/ipcsneng/neng0369.html. Accessed 2 Mar. 2017.

[14] CDC. *HEXAMETHYLENEDIAMINE*. CDC, 1 July 2014, https://www.cdc.gov/niosh/ipcsneng/neng0659.html. Accessed 2 Mar. 2017.

[15] CDC. *NITROUS OXIDE*. CDC, 1 July 2014, https://www.cdc.gov/niosh/ipcsneng/neng0659.html. Accessed 2 Mar. 2017.

[16] "Chapter 2. Polymer Synthesis." N.p.: n.p., n.d. 23-85. Print.

[17] Chaves, Ivan Dario Gil, et al. *Process Analysis and Simulation in Chemical Engineering: 2016*. Switzerland, Springer International Publishing AG, 4 Nov. 2015.

[18] Das, Tapas K. *Toward Zero Discharge: Innovative Methodology and Technologies for Process Pollution Prevention*. Hoboken, NJ: J. Wiley, 2005. Print.

[19] *Does UV Radiation Cause Cancer?* 2017, https://www.cancer.org/cancer/cancer-causes/radiation-exposure/uv-radiation/uv-radiation-does-uv-cause-cancer.html. Accessed 23 Feb. 2017.

[20] *Eco-profiles of the European Plastics Industry: Polyamide 66 (Nylon 66)*. Rep. Brussels: I Bousted for PlasticsEurope, 2005. Web.

[21] “Electric Rates.” *WKRECC*, West Kentucky Rural Electric, www.wkrecc.com/index.php/billing/electric-rates. Accessed 21 Feb. 2017.

[22] Fogler, H. Scott. *Essentials of Chemical Reaction Engineering*. Upper Saddle River, NJ: Prentice Hall, 2011. Print.

[23] Funai, Vanessa Ito, Delba Nisi Cosme Melo, Nadson Murilo Nascimento Lima, and Rubens Maciel Filho. "Simulation and Application of Response Surface Methodology to a Nylon-6 Hydrolytic Polymerization in a Semibatch Reactor." *Journal of Applied Polymer Science* 127.4 (2012): 2910-921. Web.

[24] *GPS Safety Summary*. Hexamethylenediamine. Solvay, 2012.

[25] Grossman, Lisa. *Laughing Gas Is Biggest Threat to Ozone Layer*. New Scientist, 27 Aug. 2009, https://www.newscientist.com/article/dn17698-laughing-gas-is-biggest-threat-to-ozone-layer/. Accessed 23 Feb. 2017.

[26] “Heat Transfer Coefficients Typical Values.” *Heat Transfer Coefficients Typical Values*, HC Heat Transfer, www.hcheattransfer.com/coefficients.html. Accessed 23 Feb. 2017.

[27] “INVISTIA.” *INVISTIA Performance Technologies*, ipt.invista.com/en. Accessed 1 Mar. 2017.

[28] *ISO 9000 Guidelines for the Chemical and Process Industries*. 2nd ed. Milwaukee, WI: ASQC Quality, 1996. Print.

[29] Joly, Marcel, and Jose M. Pinto. "Optimal Control of Product Quality for Batch Nylon-6,6 Autoclaves." *Chemical Engineering Journal* 97.2-3 (2004): 87-101. Web.

[30] Kaistha, Nitin, Mark S. Johnson, Charls F. Moore, and Mary G. Leitnaker. "Online Batch Recipe Adjustments for Product Quality Control Using Empirical Models: Application to a Nylon- 6,6 Process." *ISA Transactions* (2003): 305-15. Web.

[31] Mallon, Frederick K., and W. Harmon Ray. "Modeling of Solid-state Polycondensation. I. Particle Models." *Journal of Applied Polymer Science* 69.6 (1998): 1233-250. Web.

[32] Mallon, Frederick K., and W. Harmon Ray. "Modeling of Solid-state Polycondensation. II. Reactor Design Issues." *Journal of Applied Polymer Science* 69.9 (1998): 1775-788. Web.

[33] Mann, Uzi. *Principles of Chemical Reactor Analysis and Design: New Tools for Industrial Chemical Reactor Operations*. Hoboken: Wiley, 2009. Print.

[34] Mcauley, Kim B., David Berg, K. Zhen Yao, and E. Keith Marchildon. "A Dynamic Mathematical Model for Continuous Solid-phase Polymerization of Nylon 6,6." *Chemical Engineering Science* 56.16 (2001): 4801-814. Web.

[35] “Methane.” *Welcome to the NIST WebBook*, National Institute of Standards and Technology, webbook.nist.gov/cgi/cbook.cgi?ID=C74828&Mask=4. Accessed 22 Feb. 2017.

[36] “Miscellaneous Industrial Protocols Overview.” *Practical Industrial Data Networks*, 2004, pp. 402–405., doi:10.1016/b978-075065807-2/50045-5. Accessed 21 Feb. 2017.

[37] *National Oceanic and Atmospheric Administration - NOAA Study Shows Nitrous Oxide Now Top Ozone-Depleting Emission*. 27 Aug. 2009,

http://www.noaanews.noaa.gov/stories2009/20090827_ozone.html. Accessed 22 Feb. 2017.

[38] Nieschlage, HJ, J.A Rothfus, and VE Sohns, Nylon 1313 from Brassylic Acid, I and EC Product Research and Development, Vol 16, Pg 101, March 1977.

[39] *Nitrogen Oxides (NOx), Why and How They Are Controlled*, EPA, 1999, https://www3.epa.gov/ttncatc1/dir1/fnoxdoc.pdf. Accessed 2 Mar. 2017.

[40] Nylon 1313 Synthesis and Polymerization of Monomers, Journal of Polymer Science Part A-1 Vol 5 1967.

[41] *Nylon 6 and Nylon 6, 6*. O ECOTEXTILES, 5 June 2012, https://oecotextiles.wordpress.com/2012/06/05/nylon-6-and-nylon-66/. Accessed 2 Mar. 2017.

[42] *Nylon 6 and Nylon 6,6: Process Technology, Production Costs, Regional Supply/Demand Forecasts, and Economic Comparison of Alternative Production Routes Are Presented.* Publication. N.p.: Nexant, 2009. Print.

[43] *Nylon 6,6 MSDS*. Material Safety Data Sheet. Edinburgh Plastics, 2 Oct. 2007.

[44] "Nylon 6/6 (PA) – Polyamide 6/6." *RTP Company*, www.rtpcompany.com/products/product-guide/nylon-66-pa-polyamide-66/. Accessed 1 Mar. 2017.

[45] "Overview of Greenhouse Gases." *EPA*, Environmental Protection Agency, 14 Feb. 2017, www.epa.gov/ghgemissions/overview-greenhouse-gases. Accessed 25 Feb. 2017.

[46] "Paratherm™ HT Hydrogenated Terphenyl Heat Transfer Fluid." *Paratherm | Heat Transfer Fluids*, www.paratherm.com/heat-transfer-fluids/paratherm-ht-synthetic-aromatic-heat-transfer-fluid/. Accessed 22 Feb. 2017.

[47] Rau, Tiffany, Chelsea Monty, and Sarah Ewing. *AIChE 2017 Student Design Competition Problem Statement*. American Institute of Chemical Engineers, 2017. Web.

[48] Response, NOAA Office of, et al. *HEXAMETHYLENEDIAMINE, SOLUTION*. https://cameochemicals.noaa.gov/chemical/3578. Accessed 2 Mar. 2017.

[49] Riggs, James B., and M. Nazmul Karim. *Chemical and Bio-process Control*. Austin, TX: Ferret, 2016. Print.

[50] Rodriguez, Ferdinand. *Principles of Polymer Systems.* 3rd ed. N.p.: n.p., 1970. Print.

[51] Rosenthal, Jim. “Problems with Ozone Generators and Ionizers That Produce Ozone.” *Allergy Clean Environments*, 17 Feb. 2016, http://www.allergyclean.com/problems-with-ozone-generators-and-ionizers-that-produce-ozone/. Accessed 2 Mar. 2017.

[52] Russell, S.A., D.G. Robertson, J.H. Lee, and B.A. Ogunnaike. "Control of Product Quality for Batch Nylon 6,6 Autoclaves." *Chemical Engineering Science* 53.21 (1998): 3685-702. Web.

[53] “Science - Ozone Basics.” Stratospheric Ozone. *NOAA*, http://www.ozonelayer.noaa.gov/science/basics.htm. Accessed 2 Mar. 2017.

[54] Seider, W., J.D. Seader, and D.R. Lewin, Product and Process Design Principles: Synthesis, Analysis and Evaluation, Wiley, 2003.

[55] “Self Dumping Hoppers - Hoppers and Cube Trucks - Grainger Industrial Supply.” *Grainger*, 1994, https://www.grainger.com/category/self-dumping-hoppers/hoppers-and-cube-trucks/carts-and-trucks/material-handling/ecatalog/N-1221. Accessed 2 Mar. 2017.

[56] Shires, G L. “FURNACES.” *THERMOPEDIA™*, www.thermopedia.com/content/796/. Accessed 23 Feb. 2017.

[57] Sieniutycz, Stanislaw, and Jacek JezÌsowski. *Energy Optimization in Process Systems*. 1st ed. Amsterdam: Elsevier, 2009. Print.

[58] "Synthetic Fibers." *Organic Chemical Process Industry*. N.p.: EPA, n.d. N. pag. Print.

[59] Theodore, Louis. *Chemical Reactor Analysis and Applications for the Practicing Engineer.* Hoboken, NJ: Wiley, 2012. Print.

[60] “Theoretical Calculation for N2O Emission for Nylon66 Production Process.” *NSF Standards*, National Science Foundation, standards.nsf.org/apps/group_public/download.php/11153/Theoretical_. Accessed 22 Feb. 2017.

[61] “Trade Data | UN Comtrade: International Trade Statistics.” *United Nations*, United Nations, comtrade.un.org/data/. Accessed 15 Feb. 2017.

[62] Turton, Richard, Richard C. Bailie, Wallace B. Whiting, Joseph A. Shaeiwitz, and Debangsu Bhattacharyya. *Analysis, Synthesis, and Design of Chemical Processes*. 4th ed. UP, India: Pearson India Education Services, 2016. Print.

[63] "Twin Screw Extruder Pelletizer Plastic Granulator Machine Exporter/Importer,Suppliers,Factory,Manufacturers." *Cable Stripper Machine*, 25 Sept. 2016, www.cablestrippermachine.online/product/twin-screw-extruder-pelletizer-plastic-granulator-machine_23955.html. Accessed 21 Feb. 2017.

[64] Ulrich, Gael D, and Palligarnai T Vasudevan. "How to Estimate Utility Costs." *Chemical Engineering*, Apr. 2006, pp. 66–69., Accessed 23 Feb. 2017.

[65] Walas, Stanley M. *Chemical Process Equipment: Selection and Design*. Boston, Butterworth-Heinemann, 1990.

[66] Wilcox, W.R. "Cost Estimating for Chemical Engineering Plant Design." *Cost Estimating for Chemical Engineering Plant Design*, Clarkson, people.clarkson.edu/~wwilcox/Design/refcosts.htm. Accessed 21 Feb. 2017.

[67] *1,6-Hexanediamine MSDS*. Material Safety Data Sheet. ScienceLab.com, 2013.

[68] "51-8091 Chemical Plant and System Operators." *U.S. Bureau of Labor Statistics*, U.S. Bureau of Labor Statistics, www.bls.gov/oes/current/oes518091.htm. Accessed 7 Mar. 2017.

[69] *401 KAR 51: 001. Definitions for 401 KAR Chapter 51*. 20 Oct. 2010, http://www.lrc.ky.gov/kar/401/051/001.htm. Accessed 22 Feb. 2017.

Appendix

Contents

Variable Definitions
Full Aspen Optimization Tables
Batch Sensitivity Analysis
Continuous Sensitivity Analysis
Time Considerations for Process Design
Batch Process Design
Continuous Process Design
Heat Transfer Coefficients
Cost Summary
Utility Calculations
Equipment Costing Hand Calculations
Aspen Reports
Aspen HYSYS Screen Shots

Variable Definitions

Table A1. Variable Definitions

Variable	**Description, Units**
r_{fwd}	Forward reaction rate, lbmol/ft^3/s
r_{rev}	Reverse reaction rate, lbmol/ft^3/s
R	Ideal gas constant, 1.9859 BTU/°R/lbmol
T	Temperature, °R
ρ	Density, lbm/ft^3
C_p	Specific heat, BTU/lbm/ °R
V_{batch}	Required volume of batch reactor, ft^3
$\dot{Q}$	Heat added to the system, BTU/hr
$\Delta H_{rxn,i}$	Heat of reaction, BTU/hr
F	Flowrate through the reactor, lbm/hr
V_{PFR}	Volume of the PFR, ft^3
V_{CSTR}	Volume of the CSTR, ft^3
$t_{holdup,i}$	Holdup time in vessel, hr
$F_{0,i}$	Flowrate through the CSTR, lbm/hr
$H_{in,i}$	Enthalpy of inlet stream, BTU/lbm
$H_{out,i}$	Enthalpy of outlet stream, BTU/lbm
E_{in}	Energy into the system, BTU
E_{out}	Energy leaving the system, BTU
E_{gen}	Energy generated by the reaction, BTU
$C_p{}^0$	Purchase cost, USD
K_n	Purchase cost correlation coefficient
A	Purchase cost correlation size parameter, varying units
F_p	Pressure Factor
P	Design pressure of vessel, barg
D	Diameter of vessel, m
C_n	Pressure Factor correlation coefficient
C_{BM}	Bare Module cost, USD
F_{BM}	Bare Module Factor
F_T	Superheat correction factor
B_n	Bare Module Factor correlation coefficient
F_m	Material Factor
C_{TM}	Total Module cost, USD
C_{GR}	Grass Roots cost, USD
$C_{BM}{}^0$	Bare Module cost at base conditions, USD
P_{Aspen}	Pressure from simulation software, psig
f_b	Flowrate into batch reactor, m^3/hr
t_{feed}	Batch Feed time, hr
A	Heat exchanger area, m^2
Q	Heat duty of the heat exchanger, BTU/hr

U	Heat transfer coefficient, BTU/hr/ft^2/°F
$T_{H,in}$	Temperature of heating fluid in, °F
$T_{H,out}$	Temperature of heating fluid out, °F
$T_{C,in}$	Temperature of cold stream in, °F
$T_{C,out}$	Temperature of cold stream out °F
V_i	Volume of vessel, ft^3
$f_{in,i}$	Flowrate into the vessel, ft^3/hr
$t_{store,i}$	Storage time in vessel, hr
W_{belt}	Width of belt, ft
m_{belt}	Mass flowrate onto belt, lbm/hr
l_{belt}	Length of belt, ft
COM	Cost of Manufacturing, USD
FCI	Fixed Capital Investment, USD
C_{OL}	Cost of Operating Labor, USD
C_{UT}	Utility Costs, USD
C_{WT}	Waste Treatment Cost, USD
C_{RM}	Raw Material Cost, USD
P	Number of particulate processing steps
N_{np}	Number of nonparticulate processing steps
N_{OL}	Number of operators per shift
Equipment	Compressors, Exchangers, Heaters, Reactors, and Towers
RN_{OL}	Required number of operators
W_O	Hourly wage of operators, USD
W_{min}	National United States minimum wage□, USD
H_{op}	Hours operating per year, hr/year
U_{oil}	Unit cost of hot oil, USD/kJ
Q_H	Heat supplied by hot oil, kJ/s
T	Desired process temperature, K
C_{oil}	Cost of hot oil, USD
H_{fill}	Fill height of batch reactor, m
D_{batch}	Diameter of batch reactor, m
g	Gravitational constant, 9.8 m/s^2
Ap	Cross-sectional area of the exit pipe, m^2
At	Cross-sectional area of the tank, m^2
H	Height of fluid in batch reactor, m
D_{op}	Days operating in one year, day/year
t_{batch}	Batch running time, hr/day
t_{down}	Batch down time, hr
$H_{op,batch}$	Batch hours operating in one year, hr/year
$H_{op,cont}$	Continuous hours operating in one year, hr/year
DPN	Degree of polymerization

Full Aspen Optimization Tables

Please note that within these tables the acronym DNW is seen in many of the tables. This signifies that the Aspen simulation did not work with the conditions shown.

Batch

Table A2. Batch Feed Temperature Optimization

	Feed Temp to R-100				
Heater Temp (°F)	Temp (°F)	Nylon-6,6 (lb/hr)	DPN	Water Content (%)	Y/N?
290	235.425	10207.3	135.68	0.1114	Y
250	223.286	10210.1	152.327	0.1114	Y
255	224.788	10213.9	113.813	0.1116	Y
260	226.295	10207	121.889	0.1115	Y

Table A3. Batch Reactor Temperature Optimization

	R-100 Temperature			
Temp (°F)	Nylon-6,6 (lb/hr)	DPN	Water Content (%)	Y/N?
550	10213.9	113.813	0.1116	Y
520	10209.4	110.951	0.1116	Y
530	10210.7	113.823	0.1116	Y
540	10211.9	117.226	0.1115	Y
560	10207.7	129.563	0.1115	Y
570	10210.3	120.679	0.1115	Y
580	10211.7	124.009	0.1115	Y
590	10205.1	158.138	0.1114	Y

Table A4. Batch Reactor Pressure Optimization

	R-100 Pressure			
Pressure (atm)	Nylon-6,6 (lb/hr)	DPN	Water Content (%)	Y/N?
1	10199	238	0.0646	N
2	10208	168	0.1115	N
3	10207.2	145	0.1114	N
4	10208.8	132	0.1115	N
5	10213.9	113.813	0.1116	Y
6	10210.2	105	0.1116	N

Table A5. Batch Process Feed Heating

	Amount of Feed Being Heated in E-100				
%	Feed Temp (°F)	Nylon-6,6 (lb/hr)	DPN	Water Content (%)	Y/N?
29.4	224.788	10213.9	113.813	0.1116	Y
40	229.369	10204.4	157.6	0.1114	N
50	233.7	10203.4	191	0.1113	N
60	238	10208.9	123.8	0.1115	N

20	220.7	10211.3	134.8	0.1114	N

Continuous

Table A6. Continuous Process PFR Temperature

	R-200 Temperature		
Temperature (°F)	DPN	Nylon-6,6 (lb/hr) at CSTR Outlet	Y/N?
520	108.5	10217.8	Y
530	113.4	10213.9	Y
540	DNW	DNW	DNW
550	DNW	DNW	DNW

Table A7. Continuous Process PFR Pressure

	R-200 Pressure		
Pressure (atm)	DPN	Nylon-6,6 (lb/hr) at CSTR Outlet	Y/N?
3	DNW	DNW	DNW
4	DNW	DNW	DNW
5	113.4	10213.9	Y
6	101.6	10223.1	Y
7	93.16	10226.7	Y
8	86.68	10227.9	Y
9	81.4	10228.2	Y
10	76.8	10228.3	Y

Table A8. Continuous Process PFR Volume

		R-200 Volume (Assume Constant L/D=25)		
Length (ft)	Diameter (ft)	DPN	Nylon-6,6 (lb/hr) at CSTR Outlet	Y/N?
25	1	DNW	DNW	DNW
50	2	27.3	9580.6	N
100	4	97.3	10177	N
150	6	101.6	10223.1	Y
175	7	100.8	10226.8	Y
200	8	100.67	10227.5	Y
225	9	100.7	10227.6	Y

Table A9. Continuous Process Feed Heating

		Amount of Feed Being Heated		
%	Feed Temp (°F)	Nylon-6,6 (lb/hr)	DPN	Y/N?
29.4	224.8	10213.9	113.4	Y
40	229.37	10213.9	113.64	Y
50	233.7	10213.9	113.64	Y

Table A10. Continuous Process CSTR Temperature

R-201 Temperature			
Temperature (°F)	DPN	Nylon-6,6 (lb/hr) at CSTR Outlet	Y/N?
520	101.64	10224.8	Y
530	101.64	10224.5	Y
540	101.64	10224.3	Y
550	101.64	10224.1	Y
560	101.64	10223.9	Y
510	101.64	10225.1	Y

Table A11. Continuous Process CSTR Temperature

R-201 Pressure			
Pressure (atm)	DPN	Nylon-6,6 (lb/hr) at CSTR Outlet	Y/N?
4	101.64	10228	Y
3	101.64	10226.5	Y
2	101.64	10225.1	Y
3.5	101.64	10227.3	Y
2.5	101.64	10225.8	Y

Batch Sensitivity Analysis

Table A12. Variation in Parameters for Batch Sensitivity Analysis[62]

Variable	*Low Value*	*High Value*
Sales Price of Nylon-6,6	- 20%	+ 20%
Purchase Price of ADA	- 20%	+ 20%
Purchase Price of HMDA	- 20%	+ 20%
Equipment Costs	- 25%	+ 40%
Operating Costs	- 25%	+ 40%
Project Life	7 years	15 years

Table A13. Effect of Sales Price of Nylon-6,6 on Batch Project Economics

Sales Price of Nylon-6,6	***Base Case***	***- 20%***	***+ 20%***
NPV	**73,300,000**	**14,000,000**	**132,000,000**
DCFROR	**68.9%**	**29.2%**	**96.6%**

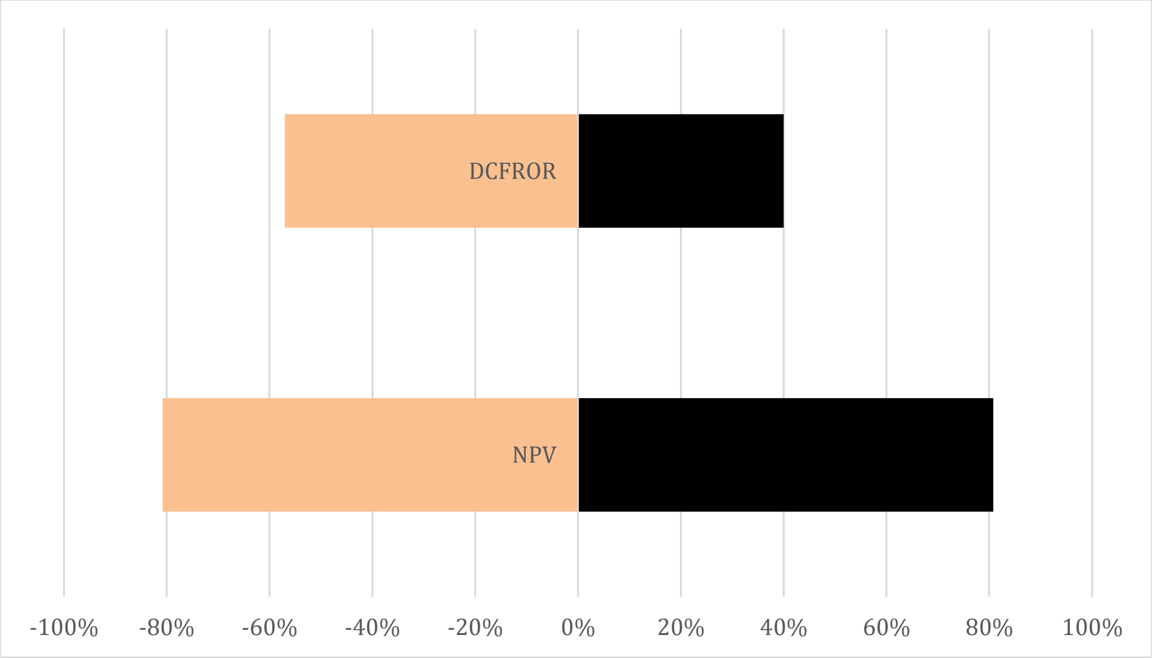


Figure A1. Effect of Sales Price of Nylon-6,6 on Batch Project Economics

Table A14. Effect of Purchase Price of ADA on Batch Project Economics

Purchase Price of ADA	***Base Case***	***- 20%***	***+ 20%***
NPV	**73,300,000**	**85,000,000**	**62,000,000**
DCFROR	**68.9%**	**74.7%**	**62.6%**

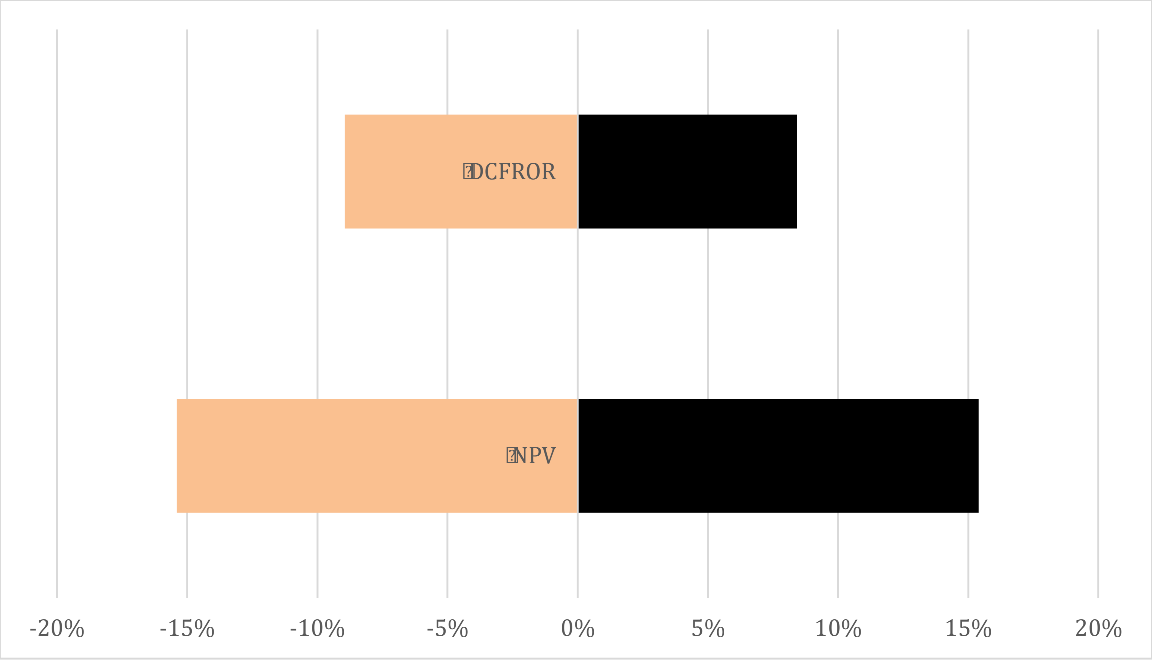


Figure A2. Effect of Purchase Price of ADA on Batch Project Economics

Table A15. Effect of Purchase Price of HMDA on Batch Project Economics

Purchase Price of HMDA	***Base Case***	***- 20%***	***+ 20%***
NPV	**73,300,000**	**89,000,000**	**58,000,000**
DCFROR	**68.9%**	**76.6%**	**60.5%**

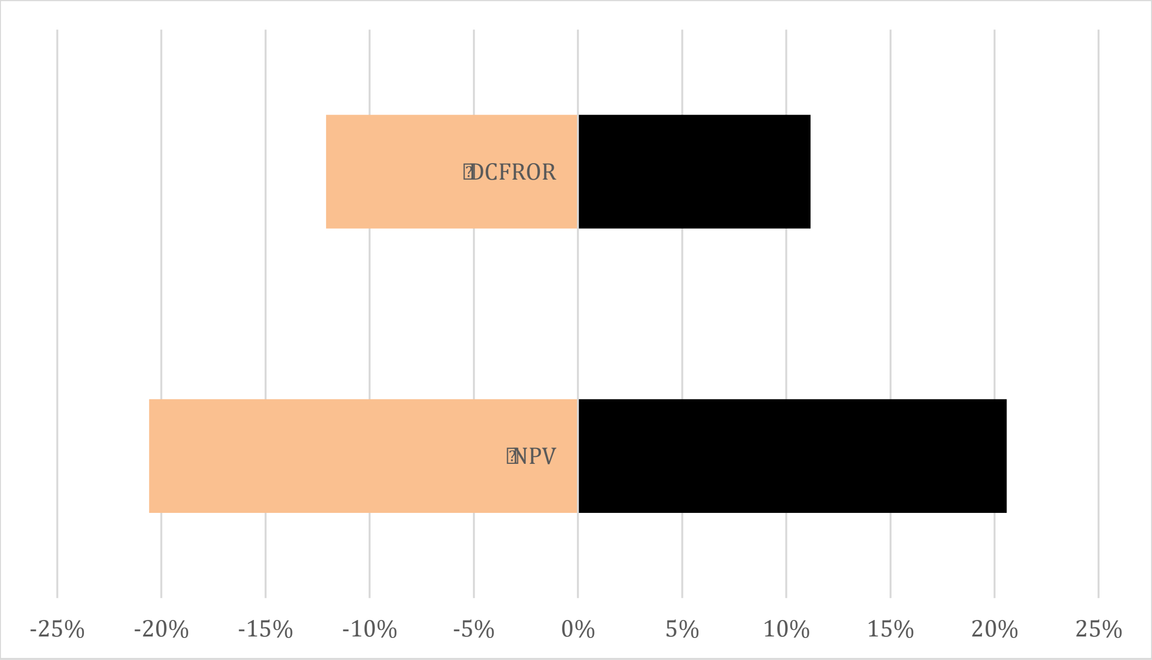


Figure A3. Effect of Purchase Price of HMDA on Batch Project Economics

Table A16. Effect of Total Equipment Cost on Batch Project Economics

Equipment Costs	***Base Case***	***- 25%***	***+ 40%***
NPV	**73,300,000**	**77,000,000**	**67,000,000**
DCFROR	**68.9%**	**83.5%**	**54.3%**

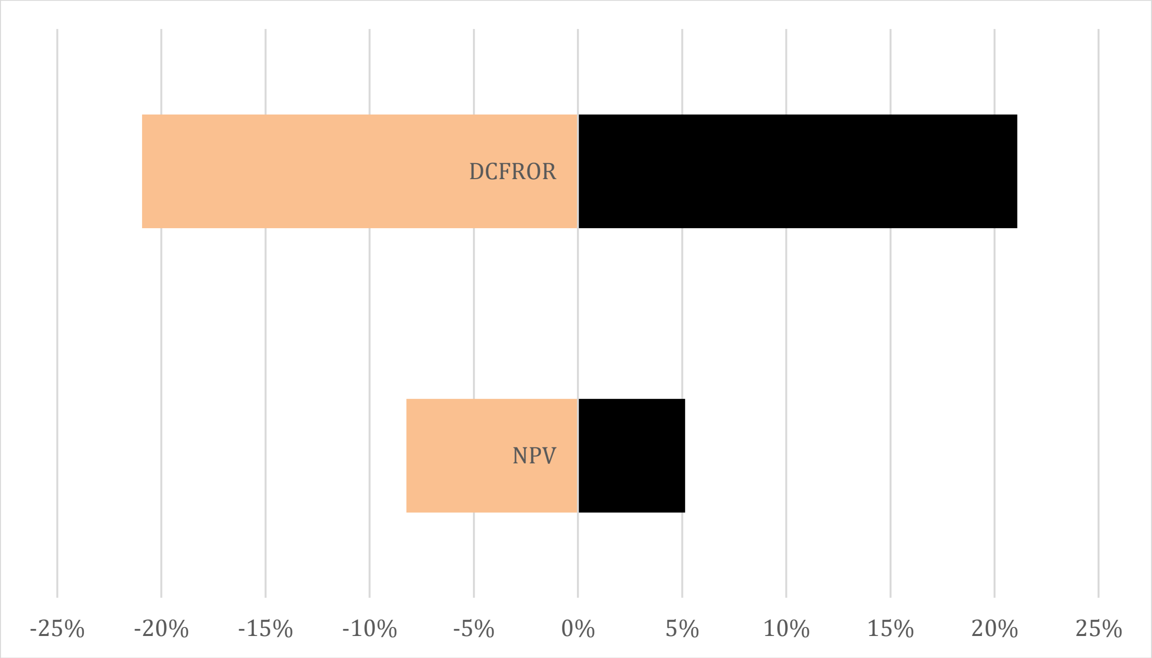


Figure A4. Effect of Total Equipment Cost on Batch Project Economics

Table A17. Effect of Operating Cost on Batch Project Economics

Operating Costs	***Base Case***	***- 25%***	***+ 40%***
NPV	**73,300,000**	**92,000,000**	**43,000,000**
DCFROR	**68.9%**	**78.5%**	**51.1%**

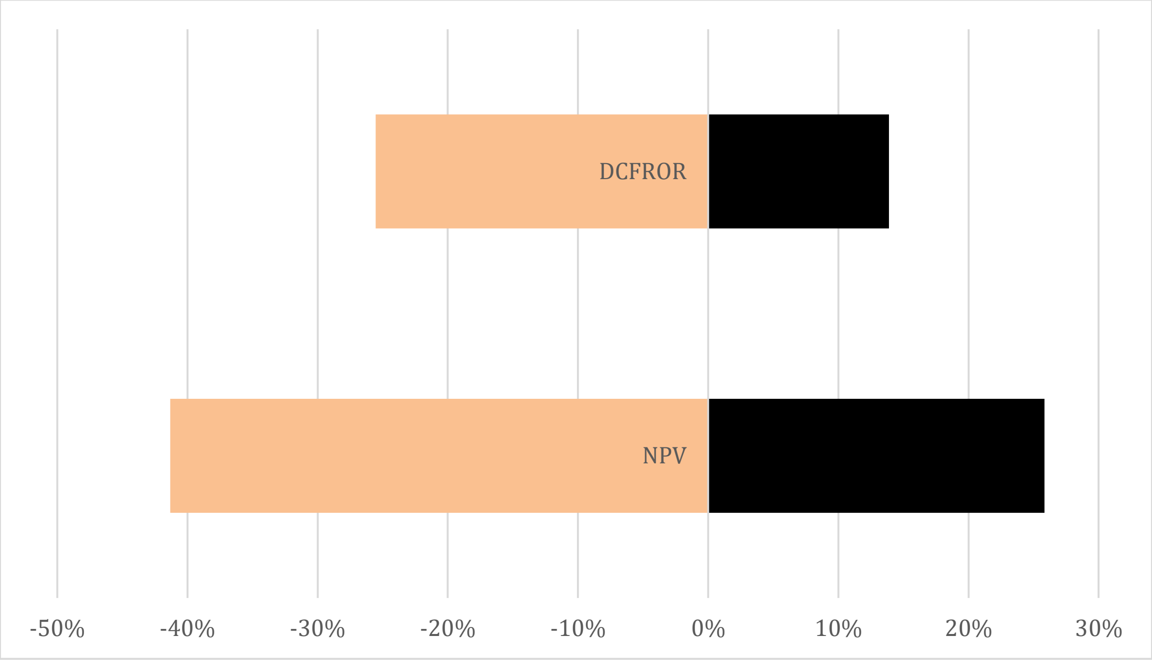


Figure A5. Effect of Operating Cost on Batch Project Economics

Table A18. Effect of Project Life on Batch Project Economics

Project Life	***Base Case (10 years)***	***7 years***	***15 years***
NPV	**73,300,000**	**53,000,000**	**93,000,000**
DCFROR	**68.9%**	**66.8%**	**69.3%**

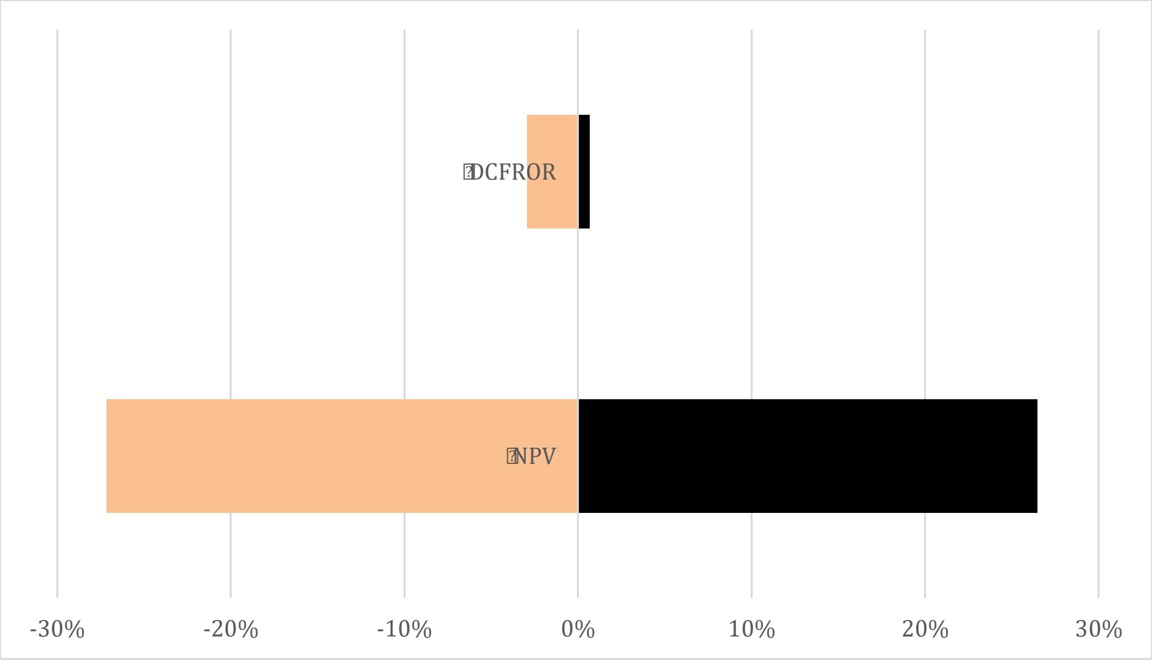


Figure A6. Effect of Project Life on Batch Project Economics

Table A19. Effect of Production Startup Time on Batch Project Economics

Startup	***Base Case (Halfway through Year 2)***	***Year 3***	***Year 4***
NPV	**73,300,000**	**64,000,000**	**49,000,000**
DCFROR	**68.9%**	**56.8%**	**43.5%**

Continuous Sensitivity Analysis

Table A20. Variation in Parameters for Continuous Sensitivity Analysis[62]

Variable	Low Value	High Value
Sales Price of Nylon-6,6	- 20%	+ 20%
Purchase Price of ADA	- 20%	+ 20%
Purchase Price of HMDA	- 20%	+ 20%
Equipment Costs	- 25%	+ 40%
Operating Costs	- 25%	+ 40%
Project Life	7 years	15 years

Table A21. Effect of Sales Price of Nylon-6,6 on Continuous Project Economics

Sales Price of Nylon-6,6	Base Case	- 20%	+ 20%
NPV	**144,000,000**	**54,600,000**	**233,000,000**
DCFROR	**117.7%**	**68.0%**	**155.5%**

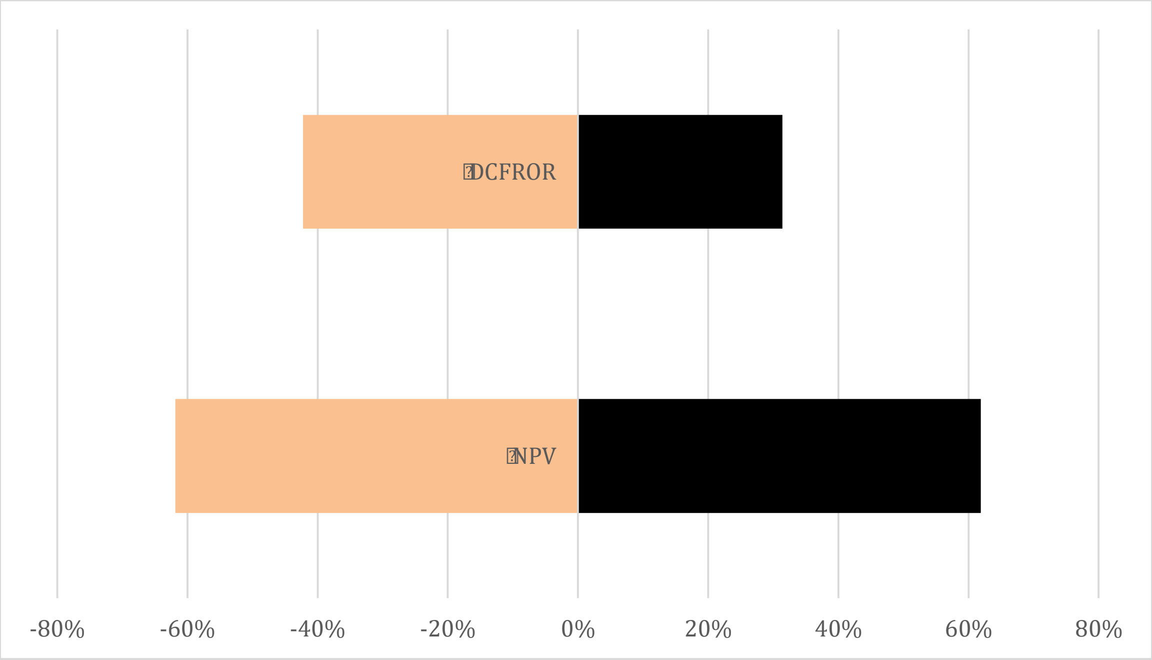


Figure A7. Effect of Sales Price of Nylon 6,6 on Continuous Project Economics

Table A22. Effect of Purchase Price of ADA on Continuous Project Economics

Purchase Price of ADA	Base Case	- 20%	+ 20%
NPV	**143,766,657**	**161,000,000**	**127,000,000**
DCFROR	**117.7%**	**126.0%**	**109.9%**

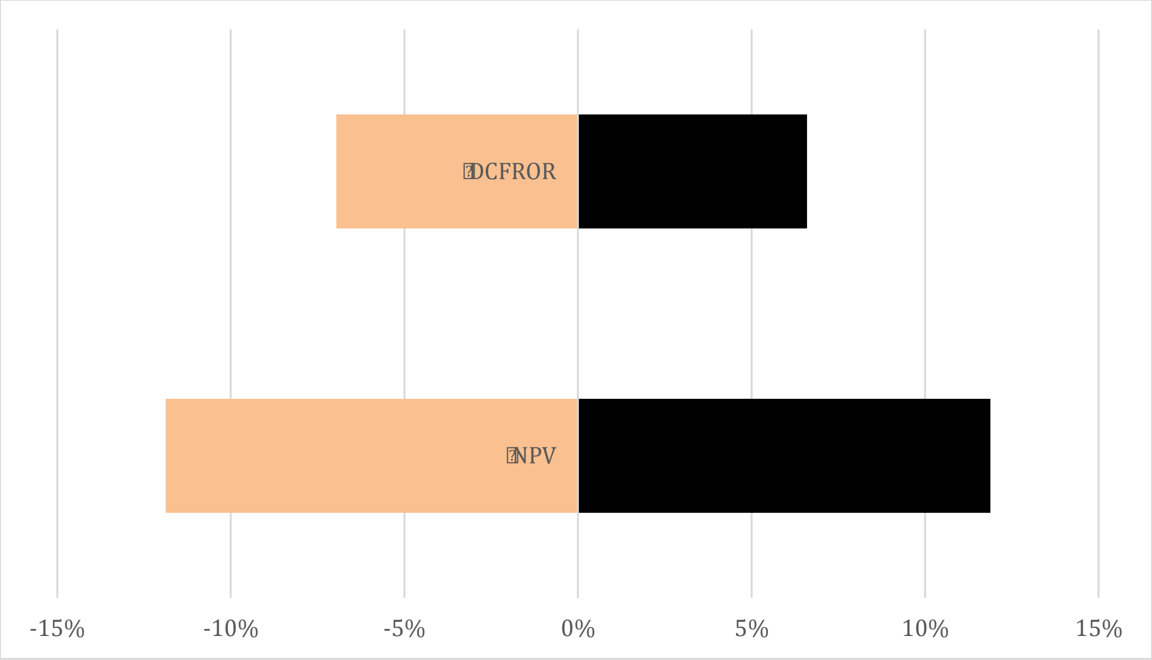


Figure A8. Effect of Purchase Price of ADA on Continuous Project Economics

Table A23. Effect of Purchase Price of HMDA on Continuous Project Economics

Purchase Price of HMDA	***Base Case***	***- 20%***	***+ 20%***
NPV	**144,000,000**	**167,000,000**	**121,000,000**
DCFROR	**117.7%**	**128.6%**	**107.1%**

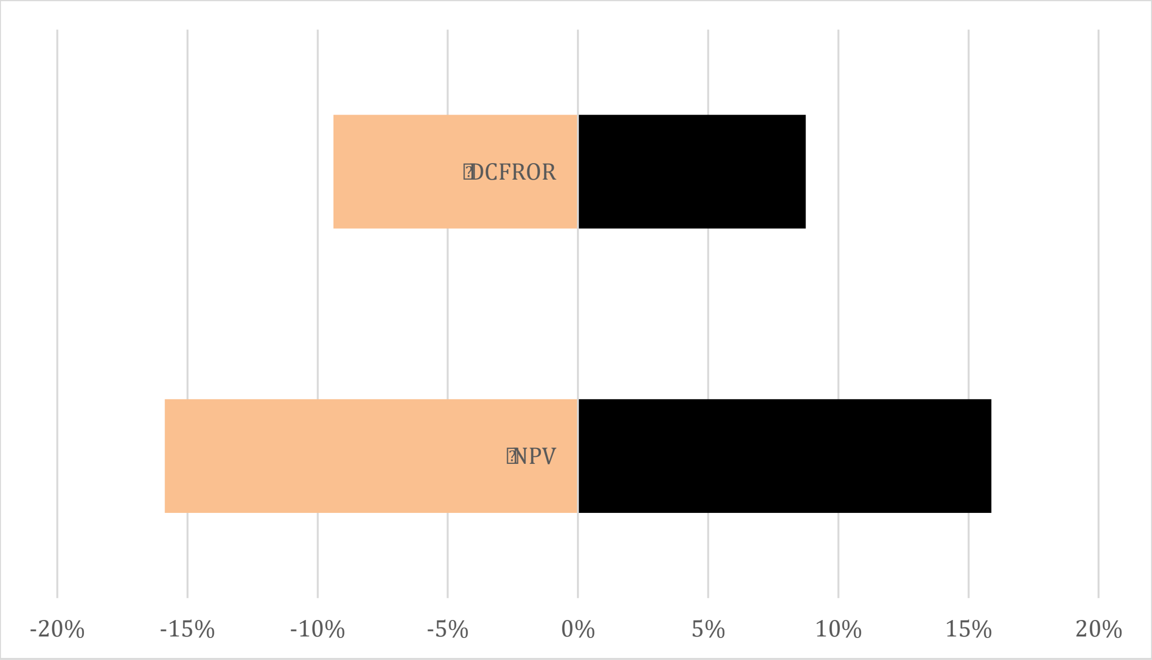


Figure A9. Effect of Purchase Price of HMDA on Continuous Project Economics

Table A24. Effect of Total Equipment Cost on Continuous Project Economics

Equipment Costs	***Base Case***	***- 25%***	***+ 40%***
NPV	**144,000,000**	**147,000,000**	**139,000,000**
DCFROR	**117.7%**	**140.9%**	**95.7%**

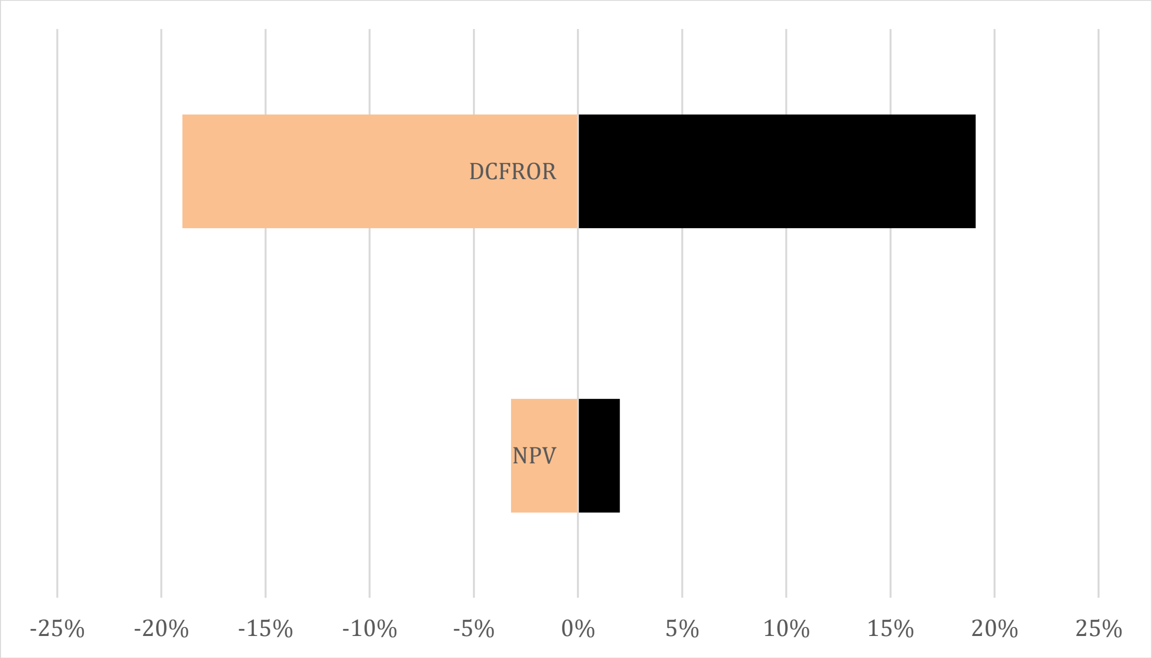


Figure A10. Effect of Total Equipment Cost on Continuous Project Economics

Table A25. Effect of Operating Costs on Continuous Project Economics

Operating Costs	***Base Case***	***- 25%***	***+ 40%***
NPV	**144,000,000**	**166,000,000**	**108,000,000**
DCFROR	**117.7%**	**128.3%**	**100.2%**

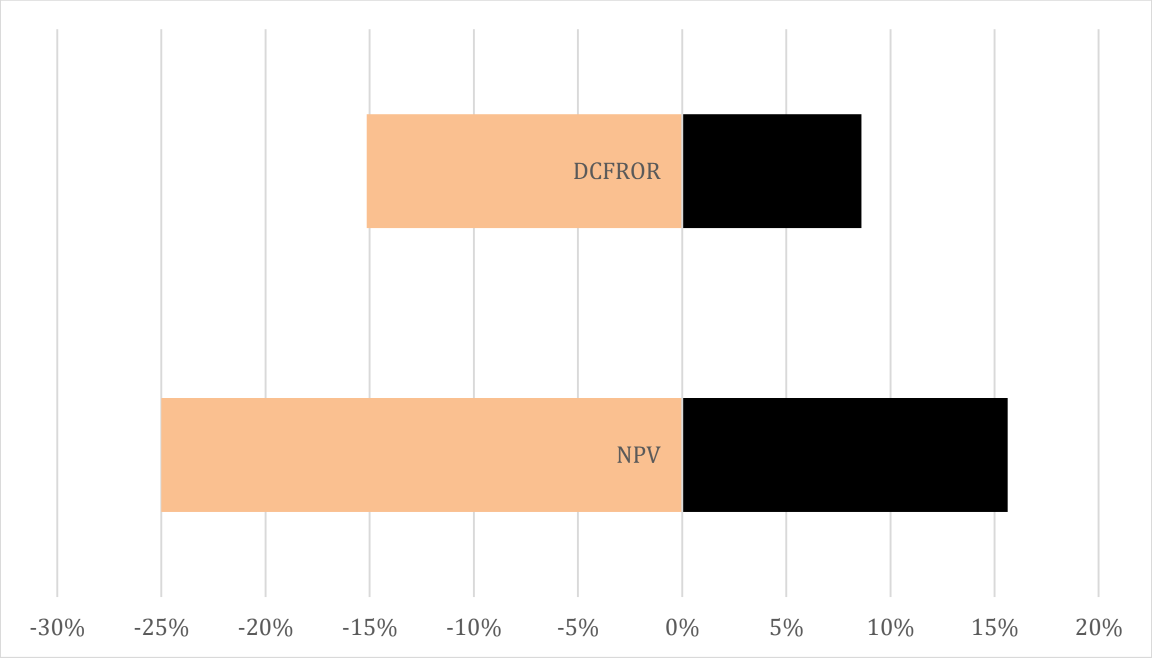


Figure A11. Effect of Operating Costs on Continuous Project Economics

Table A26. Effect of Project Life on Continuous Project Economics

Project Life	***Base Case (10 years)***	***7 years***	***15 years***
NPV	**144,000,000**	**109,000,000**	**178,000,000**
DCFROR	**117.7%**	**117.3%**	**118.2%**

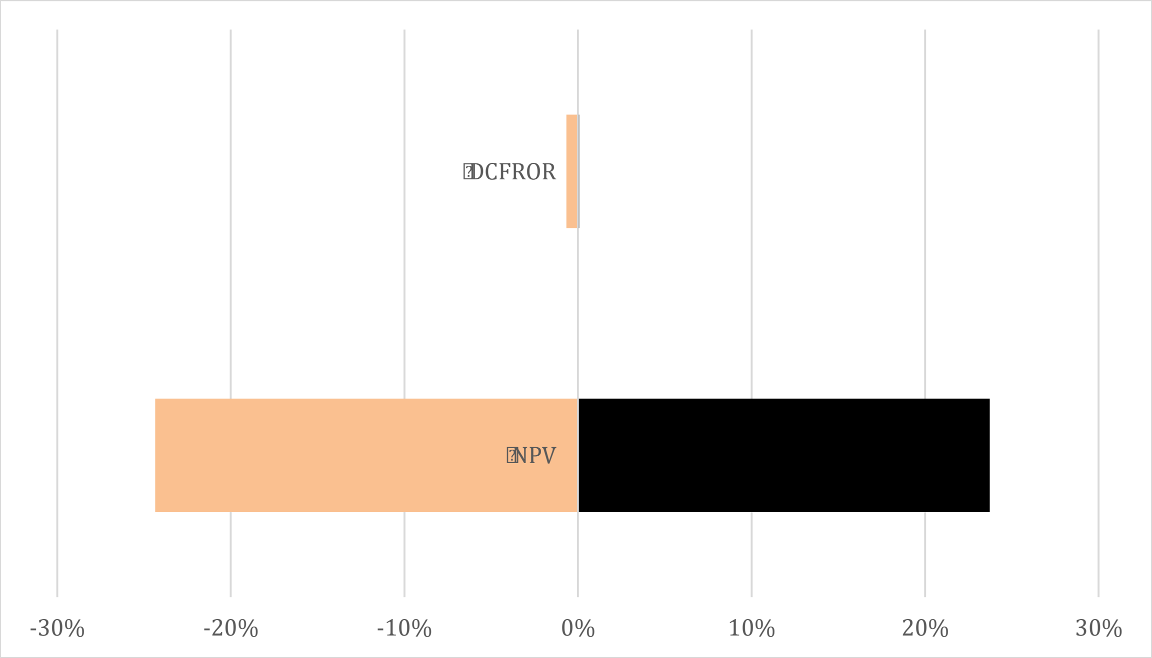


Figure A12. Effect of Project Life on Continuous Project Economics

Table A27. Effect of Production Startup Time on Continuous Project Economics

Startup	***Base Case (Halfway through Year 2)***	***Year 3***	***Year 4***
NPV	**144,000,000**	**128,000,000**	**101,000,000**
DCFROR	**117.7%**	**91.9%**	**67.6%**

Time Considerations for Process Design

Table A28. Batch and Continuous Time Calculations

Service Factor [62]	0.96
Continuous Days in Service	350.4
Continuous Hours in Service	8409.6
Batch Days in Service	233.6
Batch process hours in service (hr/yr)	5606.4
Cycle Length (hr) [17]	2
Cleaning time between cycles (hr)	1
Number times running	8
Batch process running (hr/day)	16
Fraction of Continuous process needing Hot Oil	1
Fraction of Continuous process needing CW	0
Fraction of Batch needing Hot Oil	1
Fraction of Batch needing CW	0

Table A29. Batch Reactor Vessel Design Calculations

Length (ft)	26.78
Length (m)	8.16
Diameter (ft)	8.86
Diameter (m)	2.70
Volume (ft3)	1650.35
Mass Flow (lb/hr)	29566.50
Density of Nylon Salt (lb/ft3)	59.72
Volumetric Flow (ft3/hr)	495.10
Reaction Time (h)	2.00
Volume (m3)	46.73
L/D	3.02
Maximum Pressure (psig)	108.78
Maximum Pressure (barg)	7.50

Table A30. Batch Reactor Cooling Water Calculations

Heat Duty when cooled (Btu/hr)	35622000.00
Heat Duty (MJ/hr)	37583.20
Cool 1	0.00
Cool 2	0.00
Cool 3	0.00
Cool 4	0.00
Heat Transfer Area (m2)	69.23
Maximum Pressure (psia)	108.78
Maximum Pressure (barg)	7.50

Table A31. Batch Reactor Hot Oil Heat Exchanger Calculations

Heat Duty when cooled (Btu/hr)	24409000.00
Heat Duty (MJ/hr)	25752.86
Heat 1	0.00
Heat 2	0.00
Heat 3	0.00
Heat 4	0.00
Heat Transfer Area (m2)	6926.15
DT Log Mean (F)	32.74
Maximum Pressure (psia)	108.78
Maximum Pressure (barg)	7.50

Table A32. Batch Reactor Furnace Calculations [56]

Heat Transfer Area (ft2)	15939.82
Utility In Temperature (F)	600.00
Utility Out Temperature (F)	570.00
Process Temperature Inlet (F)	223.60
Process Temperature Desired (F)	550.00
LMTD	153.13
Correction Factor	1.00
Overall Heat Transfer Coefficient (Btu/hrft2F) [26]	10.00
Specific Heat of Paratherm HT (Btu / lb F) [46]	0.60
Mass Flow of Paratherm HT (lb / hr)	1356055.56
Heat of Combustion of Methane (MJ / kg) [35]	49.95
Q furnace (MJ / h)	64382.15
Mass flow of Methane (kg / h)	1288.93
Mass flow of air	22169.63
*****Assuming 40% efficient furnace - efficiency factor** [9]	2.50

Table A33. Batch Process ADA Storage Tank Sizing

Volumetric Flowrate of ADA (ft3/hr)	77.31
Mass Flowrate of ADA (lb/hr)	6563.76
Specifc Gravity	1.36
Density of ADA (lb/ft3)	84.90
Volume (m3)	1576.20
Volume (ft3)	55663.03
Number of Storage hours	720.00

Table A34. Batch Process HMDA Storage Tank Sizing

Volumetric Flowrate of HMDA (ft3/hr)	99.45
Mass Flowrate of HMDA (lb/hr)	5262.84
Specifc Gravity	0.85
Density of HMDA (lb/ft3)	52.92
Volume (m3)	2027.57
Volume (ft3)	71602.97
Number of Storage hours	720.00

Table A35. Batch Process Water Storage Tank Sizing

Volumetric Flowrate of Water (ft3/hr)	284.07
Mass Flowrate of Water (lb/hr)	17734.00
Specifc Gravity	1.00
Density of Water (lb/ft3)	62.43
Volume (m3)	5791.68
Volume (ft3)	204531.30
Number of Storage hours	720.00

Table A36. Batch Process Pre-Feed Heater Calculations

Heat Duty (Btu/hr)	330100.00
Heat Duty (MJ/hr)	348.27
Heat Transfer Area (m2)	3.01
Utility In Temperature (F)	489.20
Utility Out Temperature (F)	489.20
Process Temperature Inlet (F)	212.00
Process Temperature Desired (F)	255.00
LMTD	255.10
Correction Factor	1.00
Overall Heat Transfer Coefficient (Btu/hrft2F) [26]	40.00
Maximum Pressure (psig)	108.78
Maximum Pressure (barg)	7.50

Table A37. Batch Process Flash Tank Calculations

Volumetric Flowrate Required (ft3/hr)	19345.43
Mass Flowrate to Flash (lb/hr)	10270.20
Density of Process Stream (lb/ft3)	0.53
Volume (m3)	45.65
Volume (ft3)	1612.12
Holdup time (hr) [62]	0.08
Length (m)	8.06
Diameter (m)	2.69
L/D	3.00
Maximum Pressure (psig)	50.00
Maximum Pressure (barg)	3.45

Table A38. Batch Process HMDA Pump Sizing

Shaft Power (kW)	0.15
Pdischarge (barg)	4.46
Pdischarge (psig)	64.69

Table A39. Batch Process Water Pump Sizing

Shaft Power (kW)	0.27
Pdischarge (barg)	4.46
Pdischarge (psig)	64.69

Table A40. Batch Process Mixer Heat Exchanger Calculations

Heat Duty (Btu/hr)	2620000.00
Heat Duty (MJ/hr)	2764.25
Heat Transfer Area (m2)	17.95
Utility In Temperature (F)	489.20
Utility Out Temperature (F)	489.20
Process Temperature Inlet (F)	80.00
Process Temperature Desired (F)	212.00
LMTD	338.93
Correction Factor	1.00
Overall Heat Transfer Coefficient (Btu/hrft2F) [26]	40.00
Maximum Pressure (psig)	64.69
Maximum Pressure (barg)	4.46

Table A41. Batch Process Stirred Vessel Calculations

Volumetric Flowrate Required (ft3/hr)	495.10
Mass Flowrate Into Stirred Vessel (lb/hr)	29566.50
Density of Nylon Salt (lb/ft3)	59.72
Volume (m3)	2.34
Volume (ft3)	82.52
Holdup time (hr) [62]	0.17
Mass in vessel (lb)	4927.75
Length (m)	2.98
Diameter (m)	1.00
L/D	2.98
Maximum Pressure (psia)	64.69
Maximum Pressure (barg)	4.46

Table A42. Batch Process Mixer Calculations

Power of Mixer (kW)	1.076
Number of Spares	1

Table A43. Batch Process Salt Pump Calculations

Shaft Power (kW)	1.65
Pdischarge (barg)	7.50
Pdischarge (psig)	108.78

Table A44. Batch Process Salt Storage Tank Calculations

Volumetric Flowrate Required (ft3/hr)	558.70
Mass Flowrate into Storage Tank (lb/hr)	29566.50
Specifc Gravity	0.85
Density of HMDA (lb/ft3)	52.92
Volume (m3)	2.64
Volume (ft3)	93.12
Holdup Time (hr) [62]	0.17
Volume/tank (m3)	2.64
Number of Storage Tanks	1.00
Length (m)	3.11
Diameter (m)	1.04
L/D	3.00
Maximum Pressure (psig)	64.69
Maximum Pressure (barg)	4.46

Table A45. Batch Process ADA Conveyor Belt Calculations [65]

Area of Conveyor (m2)	55.74
Volumetric Flowrate of ADA (ft3/hr)	77.31
Width of the belt (ft)	2.00
Length of belt (ft)	300.00

Table A46. Batch Process ADA Chute Calculations [55][66]

Inner Diameter of Chute (ft)	3.00
Volumetric Flowrate of ADA (ft3/hr)	77.31
Volumetric Flowrate of ADA (m3/hr)	2.19
Area of Conveyor (m2)	55.74
Thickness (m)	0.01
Volume on Conveyor (m3)	0.35
Low cost of Chute/foot of height	115.50
Electricity cost of Chute	1150.00
Stainless Steel Factor	0.25
Total Cost of Chute	1294.38
Height of Chute	1.00
Holdup Time (hr)	0.08
Volume of Chute (ft3)	6.44

Table A47. Batch Process Pellet Screen Calculations [62]

Area of screen (m2)	15

Table A48. Batch Process Pellet Storage Tank Calculations

Volumetric Flowrate Required (ft3/hr)	190.40
Mass Flowrate of Nylon 6,6 (lb/hr)	10213.90
Density of Product Stream (lb/ft3)	53.64
Volume (m3)	3881.90
Volume (ft3)	137087.83
Number of Storage hours	720.00

Table A49. Batch Process Molten Nylon Pump Calculations

Shaft Power (kW)	0.11
Pdischarge (barg)	7.50
Pdischarge (psig)	108.78

Table A50. Batch Process Extruder Calculations [63]

Screw Size (in)	8.00
L/D	30.00
RPM	100.00
Capacity (lb / hr)	10213.90
Capacity (kg/hr)	4632.95
Operating at % Capacity	50.00
Number Needed	3.00
Capacity of selected extruder (kg/hr)	1000.00
Number of extruders needed	5.00

Table A51. Batch Process Emergency Molten Nylon Storage Tank Calculations

Volumetric Flowrate Required (ft3/hr)	190.40
Mass Flowrate of Molten Nylon 6,6 (lb/hr)	10213.90
Density of Process Stream (lb/ft3)	53.64
Volume (m3)	129.40
Volume (ft3)	4569.59
Number of Storage hours	24.00
Volume/tank (m3)	129.40
Number of Storage Tanks	1.00
Length (m)	11.40
Diameter (m)	3.80
L/D	3.00
Maximum Pressure (psia)	64.69
Maximum Pressure (barg)	4.46

Table A52. Batch Process Nitrous Oxide Calculations [39]

Cost /ton	$650.00
Duty of NO2 Furnace (Btu/hr)	9617000
Duty of NO2 Furnace (MMBtu/yr)	53917
Duty of NO2 Furnace (J/h)	10146472135
Duty of NO2 Furnace (kJ/s)	2818
Cost /kW	$54.24
Cost	$152,873.51

Table A53. Continuous Process PFR Design Heuristic [65]

L/D	25 or larger

Table A54. Continuous Process PFR Vessel Calculations

Length (ft)	132.32
Length (m)	40.33
Diameter (ft)	3.48
Diameter (m)	1.06
Volume (m3)	35.59
L/D	38.05
Maximum Pressure (psig)	123.48
Maximum Pressure (barg)	8.51

Table A55. Continuous Process PFR Cooling Water Calculations

Heat Duty when cooled (Btu/hr)	0.00
Heat Duty (MJ/hr)	0.00
Cool 1	0.00
Cool 2	0.00
Cool 3	0.00
Cool 4	0.00
Heat Transfer Area (m2)	134.30
Maximum Pressure (psia)	123.48
Maximum Pressure (barg)	8.51

Table A56. Continuous Process PFR Hot Oil Heat Exchanger Calculations

Heat Duty when cooled (Btu/hr)	2934890.00
Heat Duty (MJ/hr)	3096.47
Heat 1	0.00
Heat 2	0.00
Heat 3	0.00
Heat 4	0.00
Heat Transfer Area (m2)	136.63
DT Log Mean (F)	39.91
Maximum Pressure (psia)	123.48
Maximum Pressure (barg)	8.51

Table A57. Continuous Process PFR Furnace Calculations [56]

Heat Transfer Area (ft2)	1762.35
Utility In Temperature (F)	600.00
Utility Out Temperature (F)	550.00
Process Temperature Inlet (F)	223.60
Process Temperature Desired (F)	530.00
LMTD	166.53
Correction Factor	1.00
Overall Heat Transfer Coefficient (Btu/hrft2F) [26]	10.00
Specific Heat of Paratherm HT (Btu / lb F) [46]	0.60
Mass Flow of Paratherm HT (lb / hr)	97829.67
Heat of Combustion of Methane (MJ / kg) [35]	49.95
Q furnace (MJ / h)	7741.18
Mass flow of Methane (kg / h)	154.98
Mass flow of air	2665.63
*****Assuming 40% efficient furnace - efficiency factor [9]**	2.50

Table A58. Continuous Process CSTR Design Heuristic [65]

L/D	1

Table A59. Continuous Process CSTR Vessel Calculations

Length (ft)	4.36
Length (m)	1.33
Diameter (ft)	4.36
Diameter (m)	1.33
Volume (ft3)	64.00
Volume (m3)	1.81
L/D	1.00
Maximum Pressure (psig)	64.69
Maximum Pressure (barg)	4.46

Table A60. Continuous Process CSTR Cooling Water Calculations

Heat Duty when cooled (Btu/hr)	0.00
Heat Duty (MJ/hr)	0.00
Cool 1	0.00
Cool 2	0.00
Cool 3	0.00
Cool 4	0.00
Heat Transfer Area (m2)	134.30
Maximum Pressure (psig)	64.69
Maximum Pressure (barg)	4.46

Table A61. Continuous Process CSTR Hot Oil Heat Exchanger Calculations

Heat Duty when cooled (Btu/hr)	20999.10
Heat Duty (MJ/hr)	22.16
Heat 1	
Heat 2	
Heat 3	
Heat 4	
Heat Transfer Area (m2)	4.19
dT Log Mean (F)	46.54
Maximum Pressure (psig)	64.69
Maximum Pressure (barg)	4.46

Table A62. Continuous Process CSTR Furnace Calculations [56]

Heat Transfer Area (ft2)	39.17
Utility In Temperature (F)	600.00
Utility Out Temperature (F)	550.00
Process Temperature Inlet (F)	510.00
Process Temperature Desired (F)	530.00
LMTD	53.61
Correction Factor	1.00
Overall Heat Transfer Coefficient (Btu/hrft2F) [26]	10.00
Specific Heat of Paratherm HT (Btu / lb F) [46]	0.60
Mass Flow of Paratherm HT (lb / hr)	699.97
Heat of Combustion of Methane (MJ / kg) [35]	49.95
Q furnace (MJ / h)	55.39
Mass flow of Methane (kg / h)	1.11
Mass flow of air	19.07
*****Assuming 40% efficient furnace - efficiency factor** [9]	2.50

Table A63. Continuous Process CSTR Mixer Calculations

Power of Mixer (kW)	1.147
Number of Spares	1

Table A64. Continuous Process ADA Storage Tank Sizing

Volumetric Flowrate of ADA (ft3/hr)	77.85
Mass Flowrate of ADA (lb/hr)	6609.21
Specifc Gravity	1.36
Density of ADA (lb/ft3)	84.90
Volume (m3)	1587.12
Volume (ft3)	56048.46
Number of Storage hours	720.00

Table A65. Continuous Process HMDA Storage Tank Sizing

Volumetric Flowrate of HMDA (ft3/hr)	100.14
Mass Flowrate of HMDA (lb/hr)	5299.27
Specifc Gravity	0.85
Density of HMDA (lb/ft3)	52.92
Volume (m3)	2041.61
Volume (ft3)	72098.62
Number of Storage hours	720.00

Table A66. Continuous Process Water Storage Tank Sizing

Volumetric Flowrate of Water (ft3/hr)	286.04
Mass Flowrate of Water (lb/hr)	17856.80
Specifc Gravity	1.00
Density of Water (lb/ft3)	62.43
Volume (m3)	5831.79
Volume (ft3)	205947.59
Number of Storage hours	720.00

Table A67. Continuous Process Pre Feed Heater Calculations

Heat Duty (Btu/hr)	565000.00
Heat Duty (MJ/hr)	596.11
Heat Transfer Area (m2)	5.14
Utility In Temperature (F)	489.20
Utility Out Temperature (F)	489.20
Process Temperature Inlet (F)	212.00
Process Temperature Desired (F)	255.00
LMTD	255.10
Correction Factor	1.00
Overall Heat Transfer Coefficient (Btu/hrft2F) [26]	40.00
Maximum Pressure (psig)	108.78
Maximum Pressure (barg)	7.50

Table A68. Continuous Process Flash Tank Calculations

Volumetric Flowrate Required (ft3/hr)	56078.44
Mass Flowrate into Flash Tank (lb/hr)	29771.20
Density of Process Stream (lb/ft3)	0.53
Volume (m3)	132.33
Volume (ft3)	4673.20
Holdup time (hr) [62]	0.08
Length (m)	11.49
Diameter (m)	3.83
L/D	3.00
Maximum Pressure (psig)	79.39
Maximum Pressure (barg)	5.47

Table A69. Continuous Process HMDA Pump Calculations

Shaft Power (kW)	0.15
Pdischarge (barg)	4.46
Pdischarge (psig)	64.69

Table A70. Continuous Process Water Pump Calculations

Shaft Power (kW)	0.28
Pdischarge (barg)	4.46
Pdischarge (psig)	64.69

Table A71. Continuous Process Mixer Heat Exchanger Calculations

Heat Duty (Btu/hr)	2639000.00
Heat Duty (MJ/hr)	2784.29
Heat Transfer Area (m2)	18.08
Utility In Temperature (F)	489.20
Utility Out Temperature (F)	489.20
Process Temperature Inlet (F)	80.00
Process Temperature Desired (F)	212.00
LMTD	338.93
Correction Factor	1.00
Overall Heat Transfer Coefficient (Btu/hrft2F) [26]	40.00
Maximum Pressure (psia)	64.69
Maximum Pressure (barg)	4.46

Table A72. Continuous Process Stirred Vessel Calculations

Volumetric Flowrate Required (ft3/hr)	498.53
Mass Flowrate Into Stirred Vessel (lb/hr)	29771.20
Density of Nylon Salt (lb/ft3)	59.72
Volume (m3)	2.35
Volume (ft3)	83.09
Holdup time (hr) [62]	0.17
Mass in vessel (lb)	4961.87
Length (m)	3.00
Diameter (m)	1.00
L/D	3.00
Maximum Pressure (psig)	64.69
Maximum Pressure (barg)	4.46

Table A73. Continuous Process Mixer Calculations

Power of Mixer (kW)	2.763
Number of Spares	1

Table A74. Continuous Process Salt Pump Calculations

Shaft Power (kW)	1.66
Pdischarge (barg)	6.49
Pdischarge (psia)	108.78

Table A75. Continuous Process Salt Storage Tank Calculations

Volumetric Flowrate Required (ft3/hr)	562.57
Mass Flowrate into Storage Tank (lb/hr)	29771.20
Specifc Gravity	0.85
Density of HMDA (lb/ft3)	52.92
Volume (m3)	2.66
Volume (ft3)	93.76
Holdup Time (hr) [62]	0.17
Volume/tank (m3)	2.66
Number of Storage Tanks	1.00
Length (m)	3.12
Diameter (m)	1.04
L/D	3.00
Maximum Pressure (psig)	64.69
Maximum Pressure (barg)	4.460279754

Table A76. Continuous Process ADA Conveyor Belt Calculations [65]

Area of Conveyor (m2)	55.74
Volumetric Flowrate of ADA (ft3/hr)	77.85
Width of the belt (ft)	2.00
Length of belt (ft)	300.00

Table A77. Continuous Process ADA Chute Calculations [55][66]

Inner Diameter of Chute (ft)	3.00
Volumetric Flowrate of ADA (ft3/hr)	77.85
Volumetric Flowrate of ADA (m3/hr)	2.20
Area of Conveyor (m2)	55.74
Thickness (m)	0.01
Volume on Conveyor (m3)	0.35
Low cost of Chute/foot of height	$115.50
Electricity cost of Chute	$1,150.00
Stainless Steel Factor	0.25
Total Cost of Chute	$1,294.38
Height of Chute	1
Holdup Time (hr)	0.083
Volume of Chute (ft3)	6.49

Table A78. Continuous Process Pellet Screen Calculations [62]

Area of screen (m2)	15

Table A79. Continuous Process Nylon Pellet Storage Tank Calculations

Volumetric Flowrate Required (ft3/hr)	189.73
Mass Flowrate of Nylon 6,6 (lb/hr)	10213.90
Density of Product Stream (lb/ft3)	53.84
Volume (m3)	3868.15
Volume (ft3)	136602.48
Number of Storage hours	720.00

Table A80. Continuous Process Molten Nylon Pump Calculations

Shaft Power (kW)	0.11
Pdischarge (barg)	7.50
Pdischarge (psig)	108.78

Table A81. Continuous Process Extruder Calculations [63]

Screw Size (in)	8.00
L/D	30.00
RPM	100.00
Capacity (lb / hr)	10213.90
Capacity (kg/hr)	4632.95
Operating at % Capacity	50.00
Number Needed	3.00
Capacity of selected extruder (kg/hr)	1000.00
Number of extruders needed	5

Table A82. Continuous Process Emergency Molten Nylon Storage Tank Sizing

Volumetric Flowrate Required (ft3/hr)	189.73
Mass Flowrate of Molten Nylon 6,6 (lb/hr)	10213.90
Density of Process Stream (lb/ft3)	53.84
Volume (m3)	128.94
Volume (ft3)	4553.42
Number of Storage hours	24.00
Volume/tank (m3)	128.94
Number of Storage Tanks	1.00
Length (m)	11.39
Diameter (m)	3.80
L/D	3.00
Maximum Pressure (psig)	64.69
Maximum Pressure (barg)	4.46

Table A83. Continuous Process Nitrous Oxide Scrubber Calculations [39]

Cost /ton	$650.00
Duty of NO2 Furnace (Btu/hr)	9617000.00
Duty of NO2 Furnace (MMBtu/yr)	80875.12
Duty of NO2 Furnace (J/h)	10146472134.65
Duty of NO2 Furnace (kJ/s)	2818.46
Cost /kW	54.24
Cost	$152,873.51

Heat Transfer Coefficients

Table A84. Heat Transfer Coefficients Used in Design Processes [26]

Fluid 1	**Fluid 2**	**Value (BTU / hr / ft2 / F)**
Molten Nylon	**Steam**	8
Molten Nylon	**Paratherm**	10
Nylon Salt	**Steam**	40
Nylon Salt	**Paratherm**	50
Water	**Steam**	250
HMDA	**Steam**	10

Cost Summary

Table A85. Raw Material Cost Used in Design Process [7][8][27][61]

	Purchase / kg	**Sell / kg**
Adipic Acid	$1.50	
HMDA	$2.50	
"Polyamides" including Nylon 6/6		$5.06

Table A86. Fixed Capital Investment Summary

Batch Fixed Capital Investment	$20,900,000
Continuous Fixed Capital Investment	$16,000,000

Table A87. Batch Process Manufacturing Cost Summary [62]

Raw Material Cost	$58,541,532
Waste Treatment Cost	$2,015.86
Wastewater flowrate (lb/hr)	19334.21367
Wastewater flowrate (g/hr)	8769851.801
Density of wastewater (g/cm3)	1
Wastewater volumetric flowrate (cm3/hr)	8769851.801
Wastewater volume/year (cm3)	49167297135
Wastewater volume (1000 m3)	49.16729714
Cost $/1000 m3 (heursitic p 213)	$41.00
Utility Cost	$4,473,269.77
Operating Labor Cost	$3,232,874.50
Number of Equipment	5
Compressors	0
Towers	1
Reactors	1
Heaters	1
Exchangers	2
Number of Processing steps	2
Number of operators/shift	11.59
Number of operators required for each shift	4.5
Operating Labor	53
Hourly Pay Rate In Kentucky	$10.88
Yearly pay Rate	$60,997.63
Cost of Manufacturing	$92,186,587.92

Table A88. Continuous Process Manufacturing Cost Summary [62]

Raw Material Cost	$88,420,230.16
Waste Treatment Cost	$3,053.77
Wastewater flowrate (lb/hr)	19525.89922
Wastewater flowrate (g/hr)	8856798.904
Density of wastewater (g/cm3)	1
Wastewater volumetric flowrate (cm3/hr)	8856798.904
Wastewater volume/year (cm3)	74482136060
Wastewater volume (1000 m3)	74.48213606
Cost $/1000 m3 (heursitic p 213)	$41.00
Utility Cost	$1,458,933.22
Operating Labor Cost	$4,849,311.74
Number of Equipment	7
Compressors	0
Towers	1
Reactors	2
Heaters	2
Exchangers	2
Number of Processing steps	2
Number of operators/shift	11.61
Number of operators required for each shift	4.5
Operating Labor	53
Hourly Pay Rate In Kentucky	$10.88
Yearly pay Rate	$91,496.45
Cost of Manufacturing	$128,275,341.74

Table A89. Batch Nitrous Oxide Scrubber Cost [39]

Flowrate of Streams going to Scrubber (lb/hr)	5.95
Flowrate of Streams going to Scrubber (ton/hr)	0.00
Flowrate of Streams going to Scrubber (ton/yr)	16.69
Cost/ton	650.00
Cost/yr	$10,848.13

Table A90. Continuous Nitrous Oxide Scrubber Cost [39]

Flowrate of Streams going to Scrubber (lb/hr)	5.91
Flowrate of Streams going to Scrubber (ton/hr)	0.00
Flowrate of Streams going to Scrubber (ton/yr)	24.87
Cost/ton	650.00
Cost/yr	$16,165.97

Table A91. Batch Process ADA Cost [27]

Flowrate required (lb/hr)	6564
Flowrate required (g/hr)	2977271
Mass required (kg)	16691775
Cost	$25,037,662.02

Table A92. Batch Process HMDA Cost [27]

Flowrate required (lb/hr)	5263
Flowrate required (g/hr)	2387184
Mass required (kg)	13383509
Cost	$33,458,771.90

Table A93. Batch Process Nylon-6,6 Revenue [61]

Flowrate produced (lb/hr)	10214
Flowrate produced (g/hr)	4632947
Mass required (kg)	25974155
Revenue	$131,329,570.19

Table A94. Continuous Process ADA Cost [27]

Flowrate required (lb/hr)	6609
Flowrate required (g/hr)	2997887
Mass required (kg)	25211032
Cost	$37,816,548.65

Table A95. Continuous Process HMDA Cost [27]

Flowrate required (lb/hr)	5299
Flowrate required (g/hr)	2403708
Mass required (kg)	20214226
Cost	$50,535,566.21

Table A96. Continuous Process Nylon-6,6 Revenue [61]

Flowrate required (lb/hr)	10214
Flowrate required (g/hr)	4632947
Mass required (kg)	38961232
Revenue	$196,994,355.29

Utility Calculations

Table A97. Utility Cost Summary [21[62][66]

Power, greater than 1000 kWh	$0.06746/kWh
Fuel Gas	$11.1/GJ
High pressure steam (sat)	$29.97/1000 kg
Med pressure steam (sat)	$29.95/1000 kg
Low pressure steam (sat)	$29.29/1000 kg
Paratherm HT	used hot oil correlation
Cooling water	$14.8/1000m3

Table A98. Batch Process Fuel Gas [62][66]

Power, MJ/h	64382
Power, GJ/hr	64
Power, GJ/yr	360952
Fuel Gas Cost (1 year)	$4,006,567.89

Table A99. Batch Process Power [21]

Power, kW	603
Power, kWh	3382150
Power Cost (1 year)	$228,159.84

Table A100. Batch Process Low Pressure Steam

Heat Duty (Btu/hr)	2950100
Heat of Vaporization of Water (Btu/lbm)	970
LPS Flowrate (lbm/hr)	3041
LPW Flowrate (lbm/yr)	17050970
LPS Flowrate (g/yr)	7734189772
LPS Flowrate (thousand kg/yr)	7734
LPS Cost (1 year)	$226,534.42

Table A101. Batch Process Hot Oil [62]

Grass-roots plant cost $/kJ heating capacity	$0.00
Heat required (kJ/s)	1288932
Temperature (K)	550
Grass-roots plant cost $/year	$1,159.50

Table A102. Batch Process Deionized Water

Water Flowrate (lb/hr)	17734
Water Flowrate (g/hr)	8044007
Water flowrate (kg/hr)	8044
Water Flowrate (1000 kg/yr)	45098
Deionized Water Cost	$45,097.92

Table A103. Continuous Process Fuel Gas [62][66]

Power, MJ/h	7797
Power, GJ/hr	8
Power, GJ/yr	65566
Fuel Gas Cost (1 year)	$727,783.01

Table A104. Continuous Process Power [21]

Power, kW	606
Power, kWh	5097175
Power Cost (1 year)	$343,855.40

Table A105. Continuous Process Low Pressure Steam

Heat Duty (Btu/hr)	3204000
Heat of Vaporization of Water (Btu/lbm)	970
LPS Flowrate (lbm/hr)	3303
LPW Flowrate (lbm/yr)	27777689
LPS Flowrate (g/yr)	12599747819
LPS Flowrate (thousand kg/yr)	12600
LPS Cost (1 year)	$369,046.61

Table A106. Continuous Process Hot Oil [62]

Grass-roots plant cost $/kJ heating capacity	$0.00
Heat required (kJ/s)	7796570
Temperature (K)	550
Grass-roots plant cost $/year	$2,082.23

Table A107. Continuous Process Deionized Water

Water Flowrate (lb/hr)	17857
Water Flowrate (g/hr)	8099708
Water flowrate (kg/hr)	8100
Water Flowrate (1000 kg/yr)	68115
Deionized Water Cost	$68,115.31

Table A108. Batch Process Extruder Calculations [63]

Power consumption/extruder (kW)	120
Number of Extruders	5
Power consumption (kW)	600

Table A109. Continuous Process Extruder Calculations [63]

Power consumption/extruder (kW)	120
Number of Extruders	5
Power consumption (kW)	600

Equipment Costing Hand Calculations

Table A110. Validation of Costing Method

	Vessel		**Heat Exchanger**		**Mixer**	
	CapCOST	**Group Calculation**	**CapCOST**	**Group Calculation**	**CapCOST**	**Group Calculation**
C_p^0	$4,780.00	$4,780.00	$15,900.00	$15,900.00	$43,800.00	$43,800.00
C_{BM}	$38,100.00	$37,900.00	$73,800.00	$73,800.00	$60,500.00	$60,500.00
C_{TM}	$45,000.00	$45,000.00	$87,100.00	$87,100.00	$71,400.00	$71,400.00
C_{GR}	$54,700.00	$54,400.00	$113,000.00	$113,000.00	$93,300.00	$93,300.00

Aspen Reports

Batch Block Report from Aspen Plus

```
      BLOCK:   B1       MODEL: FLASH2
      ------------------------------
         INLET STREAM:                BATCHOUT
         OUTLET VAPOR STREAM:         FLASHV
         OUTLET LIQUID STREAM:        FLASHL
         PROPERTY OPTION SET:         POLYNRTL    POLYMER NRTL /    REDLICH-KWONG

                  ***      MASS AND ENERGY BALANCE   ***
                  IN                                  OUT        RELATIVE DIFF.
TOTAL BALANCE

       MOLE(LBMOL/HR)    48.2070                 48.2070                  0.147394E-15
       MASS(LB/HR      )  10270.2                 10270.2                  0.177114E-15
       ENTHALPY(BTU/HR   )        -0.501951E+07   -0.505944E+07            0.789173E-02

***                        CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E               0.00000      LB/HR
PRODUCT STREAMS CO2E         0.00000      LB/HR NET
STREAMS CO2E PRODUCTION 0.00000 LB/HR UTILITIES CO2E
PRODUCTION   0.00000    LB/HR   TOTAL CO2E PRODUCTION
0.00000      LB/HR

***                            INPUT DATA   ***
TWO      PHASE  TP  FLASH
SPECIFIED TEMPERATURE F                                      540.000
SPECIFIED PRESSURE       PSIA                                 14.6959
MAXIMUM NO. ITERATIONS                                        30
CONVERGENCE TOLERANCE                                          0.000100000

                        ***  RESULTS  ***
OUTLET TEMPERATURE       F                                      540.00
OUTLET PRESSURE          PSIA                                   14.696
HEAT DUTY                BTU/HR                                -39928.
VAPOR FRACTION                                                 0.50550E-01


V-L PHASE EQUILIBRIUM :

      COMP          F(I)              X(I)            Y(I)            K(I)
      HDMA          0.13971E-03       0.10611E-03     0.77084E-03     7.2647
      ADA           0.28484E-04       0.29489E-04     0.96017E-05     0.32560
      WATER         0.63648E-01       0.13836E-01     0.99922         72.218
      NYLON-66      0.93618           0.98603         0.68576E-79     0.69548E-79
BLOCK:   B2       MODEL: FSPLIT
------------------------------
   INLET STREAM:              F1
   OUTLET STREAMS:            S1        S2
   PROPERTY OPTION SET:       POLYNRTL   POLYMER NRTL /    REDLICH-KWONG


                  ***      MASS AND ENERGY BALANCE   ***
                  IN                                  OUT        RELATIVE DIFF.
TOTAL BALANCE
```

```
MOLE(LBMOL/HR)          1074.72                        1074.72              0.00000
MASS(LB/HR          )   29566.5                        29566.5              -0.123044E-15
ENTHALPY(BTU/HR         )          -0.139396E+09       -0.139396E+09        0.00000

***                              CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E                    1762.16           LB/HR
PRODUCT STREAMS CO2E                 1762.16           LB/HR
NET STREAMS CO2E PRODUCTION          0.00000           LB/HR
UTILITIES CO2E PRODUCTION            0.00000           LB/HR
```

```
    TOTAL CO2E PRODUCTION              0.00000            LB/HR

                              ***     INPUT DATA     ***

  MASS-FLOW    (LB/HR      )              STRM=S1          FLOW=        8,692.55                KEY=  0

                               ***     RESULTS    ***

  STREAM= S1                  SPLIT=                0.29400        KEY=    0      STREAM-ORDER=      1
          S2                                        0.70600                0                         2

             BLOCK:    B3        MODEL: HEATER
------------------------------
INLET STREAM:              S1
OUTLET STREAM:             MIXF
PROPERTY OPTION SET:       POLYNRTL  POLYMER NRTL / REDLICH-KWONG

***                        MASS AND ENERGY BALANCE   ***
IN                                                   OUT         RELATIVE DIFF.
TOTAL BALANCE
       MOLE(LBMOL/HR)   315.968                     315.968             0.00000
       MASS(LB/HR      )   8692.55                     8692.55             0.00000
       ENTHALPY(BTU/HR   )        -0.409825E+08    -0.406614E+08      -0.783619E-02

***                        CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E                   518.076       LB/HR
    PRODUCT STREAMS CO2E              518.076          LB/HR
    NET STREAMS CO2E PRODUCTION       0.00000          LB/HR
    UTILITIES CO2E PRODUCTION         0.00000          LB/HR
    TOTAL CO2E PRODUCTION             0.00000          LB/HR


***                            INPUT DATA   ***
TWO       PHASE   TP  FLASH
SPECIFIED TEMPERATURE                      F                         255.000
SPECIFIED PRESSURE                         PSIA                       73.4797
MAXIMUM NO. ITERATIONS                                                 30
CONVERGENCE TOLERANCE                                                   0.000100000


                               ***   RESULTS   ***
   OUTLET TEMPERATURE        F                        255.00
   OUTLET PRESSURE           PSIA                     73.480
   HEAT DUTY                 BTU/HR                   0.32115E+06
   OUTLET VAPOR FRACTION                              0.0000



V-L PHASE EQUILIBRIUM :

      COMP             F(I)              X(I)              Y(I)              K(I)
      HDMA          0.42140E-01       0.42140E-01       0.22145E-02       0.21821E-01
      ADA           0.41791E-01       0.41791E-01       0.14506E-05       0.14413E-04
      WATER         0.91594           0.91594           0.99355           0.45041
N2O                    0.12501E-03    0.12501E-03    0.42318E-02      14.056

BLOCK:   B4       MODEL: MIXER
----------------------------
            INLET STREAMS:  S2              MIXF
            OUTLET          BATCHF
            PROPERTY        POLYNRTL    POLYMER NRTL /    REDLICH-KWONG
```

```
***                               MASS AND ENERGY BALANCE  ***
```

```
                                 IN                          OUT              RELATIVE DIFF.
    TOTAL BALANCE
    MOLE(LBMOL/HR)        1074.72                       1074.72             0.00000
    MASS(LB/HR        )   29566.5                       29566.5             0.123044E-15
    ENTHALPY(BTU/HR       )          -0.139075E+09      -0.139075E+09       -0.214289E-15

***                         CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E                    1762.16        LB/HR
PRODUCT STREAMS CO2E        1762.16         LB/HR NET
STREAMS CO2E PRODUCTION 0.00000 LB/HR UTILITIES CO2E
PRODUCTION  0.00000   LB/HR  TOTAL CO2E PRODUCTION
0.00000      LB/HR

***                             INPUT DATA  ***
TWO       PHASE      FLASH
MAXIMUM NO. ITERATIONS                                                30
CONVERGENCE TOLERANCE                                                  0.000100000
OUTLET PRESSURE      PSIA                                            73.4797

 BLOCK:  B5       MODEL: PUMP
 ----------------------------
INLET STREAM:              FLASHL
OUTLET STREAM:             S5
PROPERTY OPTION SET:       POLYNRTL  POLYMER NRTL / REDLICH-KWONG

***                         MASS AND ENERGY BALANCE  ***
IN                                                    OUT         RELATIVE DIFF.
TOTAL BALANCE
      MOLE(LBMOL/HR)    45.7702                         45.7702             0.00000
      MASS(LB/HR     )  10226.1                         10226.1             0.00000
      ENTHALPY(BTU/HR  )           -0.481553E+07      -0.480914E+07       -0.132772E-02

***                         CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E                   0.00000        LB/HR
    PRODUCT STREAMS CO2E              0.00000             LB/HR
    NET STREAMS CO2E PRODUCTION       0.00000             LB/HR
    UTILITIES CO2E PRODUCTION         0.00000             LB/HR
    TOTAL CO2E PRODUCTION             0.00000             LB/HR

                           ***  INPUT DATA  ***
OUTLET PRESSURE      PSIA                                            73.4797
DRIVER EFFICIENCY                                                     1.00000

FLASH SPECIFICATIONS: LIQUID
PHASE CALCULATION NO FLASH
PERFORMED
MAXIMUM NUMBER OF ITERATIONS                                          30
TOLERANCE                                                             0.000100000

                            ***  RESULTS  ***
VOLUMETRIC FLOW RATE      CUFT/HR                                   190.644
PRESSURE CHANGE      PSI                                             58.7838
NPSH AVAILABLE       FT-LBF/LB                                        0.0
FLUID POWER      HP                                                   0.81504
BRAKE POWER      HP                                                   2.51281
ELECTRICITY      KW                                                   1.87380
PUMP EFFICIENCY USED                                                  0.32435
NET WORK REQUIRED      HP                                             2.51281
HEAD DEVELOPED FT-LBF/LB                                            157.810

BLOCK:   B7       MODEL: MIXER
-----------------------------
```

```
INLET STREAMS:            FLASHV      WATEROUT
```

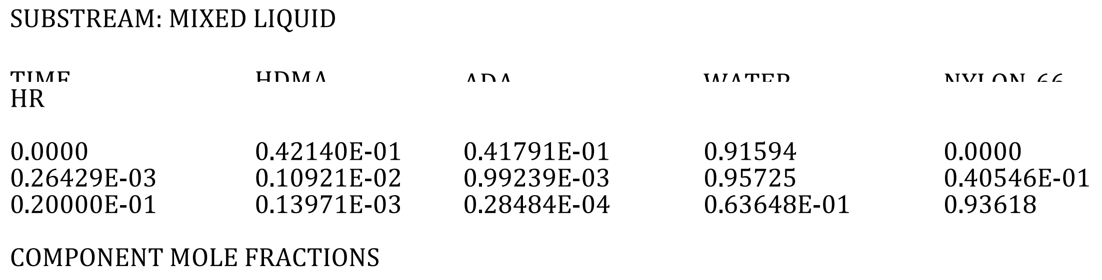
```
   OUTLET STREAM:            S7
   PROPERTY OPTION SET:      POLYNRTL    POLYMER NRTL /    REDLICH-KWONG

                  ***     MASS AND ENERGY BALANCE  ***
                  IN                               OUT        RELATIVE DIFF.
TOTAL BALANCE
```

```
        MOLE(LBMOL/HR)     1072.94                          1072.94               0.00000
        MASS(LB/HR      )  19340.4                          19340.4                    -0.188103E-15
        ENTHALPY(BTU/HR   )          -0.109568E+09      -0.109568E+09                   0.135999E-15

***                        CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E                     1762.62        LB/HR
    PRODUCT STREAMS CO2E               1762.62        LB/HR
    NET STREAMS CO2E PRODUCTION        0.00000        LB/HR
    UTILITIES CO2E PRODUCTION          0.00000        LB/HR
    TOTAL CO2E PRODUCTION              0.00000        LB/HR

***                            INPUT DATA  ***
TWO       PHASE       FLASH
MAXIMUM NO. ITERATIONS                                                 30
CONVERGENCE TOLERANCE                                                   0.000100000
OUTLET PRESSURE:     MINIMUM OF INLET STREAM PRESSURES

BLOCK:   BATCH    MODEL: RBATCH
------------------------------
   INLET STREAM:                BATCHF
   OUTLET STREAMS:              BATCHOUT    WATEROUT
   PROPERTY OPTION   SET:       POLYNRTL    POLYMER NRTL /    REDLICH-KWONG

***                        MASS AND ENERGY BALANCE  ***
IN                                          OUT       GENERATION   RELATIVE
DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)   1074.72              1118.71            43.9876              0.203246E-15
   MASS(LB/HR      )  29566.5              29566.5                                -0.520809E-07
   ENTHALPY(BTU/HR  )      -0.139075E+09   -0.114344E+09                     -0.177828

                      ***  CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E                     1762.16        LB/HR
PRODUCT STREAMS CO2E       1762.62       LB/HR NET
STREAMS CO2E PRODUCTION 0.458877 LB/HR UTILITIES
CO2E  PRODUCTION   0.00000     LB/HR   TOTAL  CO2E
PRODUCTION         0.458877      LB/HR


                        ***  INPUT DATA  ***

REACTOR TYPE:            CONSTANT  TEMPERATURE
2 PHASE: RXN IN LIQUID PHASE
DO FLASH CALCULATIONS AT EACH TIME STEP CYCLE-TIME           HR
                        3.0000
FEED-TIME               HR                                   3.0000
SET POINT TEMPERATURE F                                      550.00
INTEGRATION TOLERANCE                                        0.10000E-03
INTEGRATION METHOD                                           GEAR
CORRECTOR METHOD                                             NEWTON
VENT ALGORITHM                                               OLD

GAIN TERM FOR CONTROLLER                                     2500.0
INT-TIME TERM FOR CONTROLLER                                 0.10000E+36
DER-TIME TERM FOR CONTROLLER                                  0.0000


STOP CRITERIA

CRITERION    1 :    REACTOR     TIME
REACHES                0.20000E-01 HR                      FROM-BELOW
```

```
MAXIMUM TIME           HR                                    4.0000


                        ***  RESULTS  ***

STOP CRITERION SATISFIED                                        1
REACTION TIME                  HR                          0.20000E-01
REACTOR HEAT LOAD PER CYCLE BTU                            0.73227E+08
AVERAGE HEAT DUTY OVER CYCLE BTU/HR                         0.24409E+08
REACTOR MINIMUM TEMPERATURE F                               164.34
REACTOR MAXIMUM TEMPERATURE F                               550.53


*****                            RESULTS PROFILES  *****



** OVERALL REACTOR CONTENTS **

TIME              PRESSURE       TEMPERATURE    INST. DUTY
HR                PSIA           F              BTU/HR

0.0000             73.480         224.79        0.62008E+11
0.26429E-03        73.480         307.32        0.46238E+11
0.20000E-01        73.480         550.50       -0.33809E+08


TIME              REACTION MASS
HR                LB

   0.0000          88700.
0.26429E-03        88699.
0.20000E-01        30811.



*****                            RESULTS PROFILES  *****



** RESULTS BY SUBSTREAMS **

SUBSTREAM:   MIXED

TIME              PRESSURE       TEMPERATURE    VAPOR FRAC
HR                PSIA           F

   0.0000          73.480         224.79         0.0000
0.26429E-03        73.480         307.32        0.28379E-03
0.20000E-01        73.480         550.50         0.0000


** COMPONENT ATTRIBUTE PROFILES **

SUBSTREAM: MIXED

TIME              NYLON-66       NYLON-66       NYLON-66       NYLON-66
HR                SFRAC          SFRAC          SFRAC          SFRAC
HDMA-E                           ADA-E          HDMA-R         ADA-R
```

```
 0.0000         0.0000          0.0000              0.0000          0.0000
 0.26429E-03    0.14070         0.13467             0.36081         0.36382
 0.20000E-01    0.12094E-01     0.54791E-02         0.48956         0.49287

** COMPONENT ATTRIBUTE PROFILES **

SUBSTREAM: MIXED

 TIME           NYLON-66        NYLON-66        NYLON-66        NYLON-66
 HR             SFLOW           SFLOW ADA-E     SFLOW HDMA-     SFLOW ADA-R
                HDMA-E                          R

 0.0000         0.0000                0.0000          0.0000          0.0000
 0.26429E-03    16.828                16.107          43.154          43.515
 0.20000E-01    1.4857               0.67311          60.143          60.549

** COMPONENT ATTRIBUTE PROFILES **

SUBSTREAM: MIXED

 TIME           NYLON-66        NYLON-66        NYLON-66        NYLON-66
 HR             EFRAC           EFRAC ADA-E     ZMOM ZMOM       FMOM FMOM
                HDMA-E

 0.0000              0.0000           0.0000          0.0000          0.0000
 0.26429E-03        0.51094          0.48906          16.468          119.60
 0.20000E-01        0.68821          0.31179          1.0794          122.85

** COMPONENT ATTRIBUTE PROFILES **

SUBSTREAM: MIXED

 TIME           NYLON-66        NYLON-66
 HR             DPN             MWN
                DPN             MWN

 0.0000         0.0000                0.0000
 0.26429E-03    7.2630                839.57
 0.20000E-01    113.81                12891.

** COMPONENT MASS AMOUNTS **


SUBSTREAM: MIXED

TIME             HDMA            ADA             WATER           NYLON-66
HR               LB              LB              LB              LB

 0.0000         15789.                19691.          53202.          0.0000
 0.26429E-03    421.57                481.73          57298.          30480.
 0.20000E-01    2.3480               0.60201          165.83          30642.

SUBSTREAM: MIXED

TIME             N2O
HR               LB
```

```
  0.0000         17.740
0.26429E-03      17.740
0.20000E-01      0.0000


** RESULTS BY SUBSTREAMS **


** COMPONENT MOLE FRACTIONS ** COMPONENT MOLE FRACTIONS


SUBSTREAM: MIXED

TIME             HDMA           ADA            WATER          NYLON-66
HR

0.0000           0.42140E-01    0.41791E-01    0.91594         0.0000
0.26429E-03      0.10919E-02    0.99211E-03    0.95726        0.40535E-01
0.20000E-01      0.13971E-03    0.28484E-04    0.63648E-01    0.93618

COMPONENT MOLE FRACTIONS


SUBSTREAM: MIXED

TIME             N2O
HR

0.0000           0.12501E-03
0.26429E-03      0.12131E-03
0.20000E-01       0.0000


** RESULTS BY SUBSTREAMS **


** LIQUID PHASE MOLE FRACTIONS ** COMPONENT MOLE FRACTIONS
```



```
SUBSTREAM: MIXED LIQUID

TIME             HDMA           ADA            WATER          NYLON-66
HR

0.0000           0.42140E-01    0.41791E-01    0.91594        0.0000
0.26429E-03      0.10921E-02    0.99239E-03    0.95725        0.40546E-01
0.20000E-01      0.13971E-03    0.28484E-04    0.63648E-01    0.93618

COMPONENT MOLE FRACTIONS
```

```
SUBSTREAM: MIXED LIQUID

TIME             N2O
HR

  0.0000         0.12501E-03
0.26429E-03      0.12079E-03
0.20000E-01       0.0000
```

```
** RESULTS BY SUBSTREAMS **


** VAPOR PHASE                         MOLE FRACTIONS **

COMPONENT MOLE FRACTIONS


SUBSTREAM: MIXED VAPOR

TIME             HDMA             ADA              WATER            NYLON-66
HR

0.0000
0.26429E-03      0.65458E-04      0.12861E-06      0.99796          0.10819E-82
0.20000E-01

COMPONENT MOLE FRACTIONS


SUBSTREAM: MIXED VAPOR

TIME             N2O
HR

0.0000
0.26429E-03      0.19740E-02
0.20000E-01



** VENT ACCUMULATOR PROFILES **



    TIME         PRESSURE              TEMPERATURE          VAPOR     FRAC
    HR           PSIA                  F

0.0000
0.26429E-03
0.20000E-01              73.480            313.41              1.0000


VENT ACCUMULATOR TOTAL MASS PROFILE

TIME                     TOTAL MASS
HR                       LB

0.0000                   0.0000
0.26429E-03              0.0000
0.20000E-01              57889.



VENT ACCUMULATOR MOLE FRACTION PROFILE TIME   HDMA           ADA
                  WATER          N2O HR

0.0000             0.0000         0.0000         0.0000         0.0000
0.26429E-03        0.0000         0.0000         0.0000         0.0000
0.20000E-01       0.70313E-04    0.18492E-06    0.99980        0.12554E-03
```

```
** VENT STREAM PROFILES **


    TIME        PRESSURE            TEMPERATURE              FLOWRATE
    HR          PSIA                F                        LBMOL/HR

0.0000
0.26429E-03
0.20000E-01           73.480           550.50           0.0000

** VENT MOLE FRACTION PROFILE **


TIME            HDMA           ADA            WATER          NYLON-66 HR

0.0000
0.26429E-03
0.20000E-01     0.23548E-03    0.23564E-05    0.99976        0.85577E-81
```

Continuous Block Report from Aspen Plus

```
BLOCK: B1 MODEL: FLASH2
------------------------------ INLET STREAM: PFRO OUTLET VAPOR STREAM: FLASHV
  OUTLET LIQUID STREAM:  FLASHL


~APD07C.tmp


   PROPERTY OPTION SET: POLYNRTL POLYMER NRTL / REDLICH-KWONG

                      *** MASS AND ENERGY BALANCE  ***
                                  IN OUT RELATIVE DIFF.


    TOTAL BALANCE

       MOLE(LBMOL/HR)            1126.39         1126.39         0.00000
       MASS(LB/HR  )             29771.2         29771.2       -0.488792E-15
       ENTHALPY(BTU/HR  )  -0.113360E+09     -0.113285E+09    -0.657736E-03

                      *** CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E 1774.36  LB/HR

    PRODUCT STREAMS CO2E          1774.36      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                          ***  INPUT DATA  ***
   TWO PHASE TP  FLASH
   SPECIFIED TEMPERATURE F                                  530.000
   SPECIFIED PRESSURE  PSIA                                  44.0878
   MAXIMUM NO. ITERATIONS                                    30
   CONVERGENCE TOLERANCE                                      0.000100000

                           ***  RESULTS  ***
   OUTLET TEMPERATURE F  530.00
   OUTLET PRESSURE PSIA  44.088
   HEAT DUTY             BTU/HR                                74561.
   VAPOR FRACTION                                             0.95804

   V-L PHASE EQUILIBRIUM :

      COMP             F(I)          X(I)          Y(I)          K(I)
      HDMA           0.60698E-03   0.27406E-03   0.62157E-03    2.2680
      ADA            0.21163E-04   0.15979E-03   0.15091E-04   0.94442E-01
      WATER          0.95917       0.44334E-01   0.99924        22.539
      NYLON-66       0.40086E-01   0.95523       0.60309E-80   0.63135E-80
      N2O            0.12010E-03   0.12074E-05   0.12531E-03    103.78
 BLOCK: B2 MODEL: MIXER
 -----------------------------
   INLET STREAMS: WATER  FLASHV
   OUTLET STREAM:  N2OSCRUB
   PROPERTY OPTION SET: POLYNRTL POLYMER NRTL / REDLICH-KWONG

                      *** MASS AND ENERGY BALANCE  ***
                                  IN OUT RELATIVE DIFF.
```

```
    TOTAL BALANCE
       MOLE(LBMOL/HR)             1080.22         1080.22         0.00000
       MASS(LB/HR  )              19531.9         19531.9        0.186258E-15
       ENTHALPY(BTU/HR  )  -0.108240E+09       -0.108240E+09    -0.413003E-15

                      *** CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E              1774.20      LB/HR
    PRODUCT STREAMS CO2E           1774.20      LB/HR
    NET STREAMS CO2E PRODUCTION    0.00000      LB/HR



                                  ~APD07C.tmp

    UTILITIES CO2E PRODUCTION      0.00000      LB/HR
    TOTAL CO2E PRODUCTION          0.00000      LB/HR

                          *** INPUT DATA  ***
   TWO PHASE  FLASH
   MAXIMUM NO. ITERATIONS                                       30
   CONVERGENCE TOLERANCE                                         0.000100000
   OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

 BLOCK: B3 MODEL: PUMP
 ----------------------------

   INLET STREAM:           CSTRO
   OUTLET STREAM:          12
   PROPERTY OPTION SET:    POLYNRTL  POLYMER NRTL / REDLICH-KWONG


TOTAL BALANCE


*** MASS AND ENERGY BALANCE  ***
          IN OUT RELATIVE DIFF.

       MOLE(LBMOL/HR)             46.5101         46.5101         0.00000
       MASS(LB/HR  )              10239.3         10239.3       -0.177648E-15
       ENTHALPY(BTU/HR  )  -0.502445E+07       -0.501966E+07    -0.953283E-03

                      *** CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E 0.160047 LB/HR PRODUCT STREAMS
    CO2E 0.160047 LB/HR NET STREAMS CO2E PRODUCTION
    0.00000 LB/HR UTILITIES CO2E PRODUCTION 0.00000
    LB/HR TOTAL CO2E PRODUCTION 0.00000  LB/HR

                          ***  INPUT DATA  ***
    OUTLET PRESSURE PSIA  73.4797
    DRIVER EFFICIENCY  1.00000

    FLASH SPECIFICATIONS:
    LIQUID PHASE
    CALCULATION NO FLASH
    PERFORMED
    MAXIMUM NUMBER OF ITERATIONS  30
    TOLERANCE  0.000100000

                           ***  RESULTS  ***
    VOLUMETRIC FLOW RATE CUFT/HR  190.198
    PRESSURE CHANGE PSI  44.0878
    NPSH AVAILABLE FT-LBF/LB  0.0
    FLUID POWER HP  0.60985
    BRAKE POWER HP  1.88243
    ELECTRICITY KW  1.40373
```

```
   PUMP EFFICIENCY USED  0.32397
   NET WORK REQUIRED HP  1.88243
   HEAD DEVELOPED FT-LBF/LB  117.928

BLOCK: B4 MODEL: HEATER
------------------------------
  INLET STREAM:  12
  OUTLET STREAM:  S5
  PROPERTY OPTION SET:   POLYNRTL  POLYMER NRTL / REDLICH-KWONG

                      *** MASS AND ENERGY BALANCE  ***
                                    IN       OUT      RELATIVE DIFF.


   TOTAL BALANCE

      MOLE(LBMOL/HR)             46.5101          46.5101          0.00000
      MASS(LB/HR  )              10239.3          10239.3          0.00000
      ENTHALPY(BTU/HR  )  -0.501966E+07       -0.703707E+07     0.286684



                                             ~APD07C.tmp
                      *** CO2 EQUIVALENT SUMMARY ***

   FEED STREAMS CO2E             0.160047      LB/HR
   PRODUCT STREAMS CO2E          0.160047      LB/HR
   NET STREAMS CO2E PRODUCTION    0.00000      LB/HR
   UTILITIES CO2E PRODUCTION      0.00000      LB/HR
   TOTAL CO2E PRODUCTION          0.00000      LB/HR

                          *** INPUT DATA  ***
  TWO PHASE TP  FLASH


  SPECIFIED TEMPERATURE F  200.000
  SPECIFIED PRESSURE PSIA  73.4797
  MAXIMUM NO. ITERATIONS  30
  CONVERGENCE TOLERANCE  0.000100000



                           ***  RESULTS  ***

  OUTLET TEMPERATURE    F                                      200.00
  OUTLET PRESSURE       PSIA                                   73.480
  HEAT DUTY             BTU/HR                               -0.20174E+07
  OUTLET VAPOR FRACTION                                        0.0000


  V-L PHASE EQUILIBRIUM :


     COMP             F(I)           X(I)           Y(I)           K(I)
     HDMA            0.11396E-04    0.11396E-04    0.15331E-04    0.87372E-02
     ADA             0.85337E-04    0.85337E-04    0.18163E-07    0.13822E-05
     WATER           0.29564E-01    0.29564E-01    0.99934        0.21953
     NYLON-66        0.97034        0.97034        0.79959E-78    0.53516E-80
     N2O             0.26236E-06    0.26236E-06    0.64528E-03     15.973
BLOCK: B6 MODEL: FSPLIT
------------------------------

  INLET STREAM:          6
  OUTLET STREAMS:        S1           S2
  PROPERTY OPTION SET:   POLYNRTL  POLYMER NRTL / REDLICH-KWONG
```

```
TOTAL BALANCE


*** MASS AND ENERGY BALANCE  ***
          IN OUT RELATIVE DIFF.

       MOLE(LBMOL/HR)            1082.16         1082.16         0.00000
       MASS(LB/HR  )             29771.2         29771.2       -0.122198E-15
       ENTHALPY(BTU/HR  )  -0.140361E+09      -0.140361E+09     0.00000

                      *** CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E 1774.36  LB/HR

    PRODUCT STREAMS CO2E          1774.36      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                          *** INPUT DATA  ***

  MASS-FLOW (LB/HR ) STRM=S1 FLOW= 14,835.0 KEY= 0

                           ***  RESULTS  ***
  STREAM= S1                                             KEY=  0    STREAM-ORDER=   1
                         SPLIT=          0.49830
          S2                             0.50170           0                     2

 BLOCK: B7 MODEL: HEATER


------------------------------ INLET STREAM:  S1
  OUTLET STREAM:  MIXF

~APD07C.tmp


   PROPERTY OPTION SET: POLYNRTL POLYMER NRTL / REDLICH-KWONG

                      *** MASS AND ENERGY BALANCE  ***
                                    IN OUT RELATIVE DIFF.


    TOTAL BALANCE

       MOLE(LBMOL/HR)            539.242         539.242         0.00000
       MASS(LB/HR  )             14835.0         14835.0        0.122615E-15
       ENTHALPY(BTU/HR  )  -0.699421E+08      -0.693940E+08    -0.783619E-02

                      *** CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E 884.166  LB/HR

    PRODUCT STREAMS CO2E          884.166      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.00000      LB/HR

                          *** INPUT DATA  ***
   TWO PHASE TP  FLASH


   SPECIFIED TEMPERATURE F  255.000
   SPECIFIED PRESSURE PSIA  73.4797
   MAXIMUM NO. ITERATIONS  30
   CONVERGENCE TOLERANCE  0.000100000
```

```
                     ***  RESULTS  ***

   OUTLET TEMPERATURE    F                                   255.00
   OUTLET PRESSURE       PSIA                                73.480
   HEAT DUTY             BTU/HR                             0.54808E+06
   OUTLET VAPOR FRACTION                                     0.0000


   V-L PHASE EQUILIBRIUM :


      COMP             F(I)          X(I)          Y(I)          K(I)
      HDMA            0.42140E-01   0.42140E-01   0.22145E-02   0.21821E-01
      ADA             0.41791E-01   0.41791E-01   0.14506E-05   0.14413E-04
      WATER           0.91594       0.91594       0.99355       0.45041
      N2O 0.12501E-03 0.12501E-03 0.42318E-02  14.056

 BLOCK: B10 MODEL: MIXER
 ----------------------------
   INLET STREAMS: MIXF  S2
   OUTLET STREAM:  PFRF
   PROPERTY OPTION SET: POLYNRTL POLYMER NRTL / REDLICH-KWONG

                  *** MASS AND ENERGY BALANCE  ***
                              IN OUT RELATIVE DIFF.


    TOTAL BALANCE
       MOLE(LBMOL/HR)            1082.16         1082.16         0.00000
       MASS(LB/HR  )             29771.2         29771.2         0.00000
       ENTHALPY(BTU/HR  )  -0.139813E+09      -0.139813E+09     0.00000

                  *** CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E            1774.36      LB/HR
    PRODUCT STREAMS CO2E         1774.36      LB/HR
    NET STREAMS CO2E PRODUCTION  0.00000      LB/HR
    UTILITIES CO2E PRODUCTION    0.00000      LB/HR
    TOTAL CO2E PRODUCTION        0.00000      LB/HR




TWO PHASE  FLASH

          ~APD07C.tmp

*** INPUT DATA  ***


   MAXIMUM NO. ITERATIONS  30
   CONVERGENCE TOLERANCE  0.000100000
   OUTLET PRESSURE PSIA  73.4797

 BLOCK: CSTR MODEL: RCSTR
 ----------------------------
   INLET STREAM:  FLASHL
   OUTLET STREAMS: CSTRO  WATER
   PROPERTY OPTION SET: POLYNRTL POLYMER NRTL / REDLICH-KWONG

                  *** MASS AND ENERGY BALANCE  ***
                        IN OUT GENERATION RELATIVE DIFF.


   TOTAL BALANCE
   MOLE(LBMOL/HR) 47.2681 47.6078 0.339785  0.00000
```

```
  MASS(LB/HR  )           10259.1      10259.1                      0.177305E-15
  ENTHALPY(BTU/HR  )  -0.515549E+07  -0.513450E+07                 -0.407315E-02

                      *** CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E 0.748570 LB/HR PRODUCT STREAMS
   CO2E 0.748570 LB/HR NET STREAMS CO2E PRODUCTION
   0.00000 LB/HR UTILITIES CO2E PRODUCTION 0.00000
   LB/HR TOTAL CO2E PRODUCTION 0.00000  LB/HR

                          *** INPUT DATA ***

   REACTOR TYPE: TEMP SPEC TWO PHASE REACTOR



   REACTOR VOLUME                      CUFT                        63.990
   REACTOR TEMPERATURE                 F                           530.00
   REACTOR PRESSURE                    PSIA                        29.392

                           ***  RESULTS  ***


   REACTOR HEAT DUTY                   BTU/HR                      20999.
   RESIDENCE TIME                      HR                         0.10941
   VAPOR PHASE VOLUME FRACTION                                    0.67481
   VAPOR PHASE VOLUME                  CUFT                        43.181
   LIQUID PHASE VOLUME                 CUFT                        20.809

BLOCK: PFR MODEL: RPLUG
-----------------------------
  INLET STREAM:  PFRF
  OUTLET STREAM:  PFRO
  PROPERTY OPTION SET: POLYNRTL POLYMER NRTL / REDLICH-KWONG

                      *** MASS AND ENERGY BALANCE  ***
                              IN OUT GENERATION RELATIVE DIFF.

  TOTAL BALANCE
  MOLE(LBMOL/HR)          1082.16      1126.39      44.2247     -0.201861E-15
  MASS(LB/HR  )           29771.2      29771.2                  -0.106923E-12
  ENTHALPY(BTU/HR  )  -0.139813E+09  -0.113360E+09              -0.189204

                      *** CO2 EQUIVALENT SUMMARY ***

   FEED STREAMS CO2E              1774.36      LB/HR
   PRODUCT STREAMS CO2E           1774.36      LB/HR
   NET STREAMS CO2E PRODUCTION    0.00000      LB/HR
   UTILITIES CO2E PRODUCTION      0.00000      LB/HR
   TOTAL CO2E PRODUCTION          0.00000      LB/HR



 REACTOR TYPE:

           ~APD07C.tmp

 *** INPUT DATA  ***


    SPECIFIED TEMPERATURE

    TWO-PHASE
  REACTOR TUBE LENGTH                    FT                    132.32
  REACTOR DIAMETER                       FT                    3.4777
```

```
REACTOR RISE                         FT                    0.0000
NUMBER OF REACTOR TUBES                                    1
REACTOR VOLUME                       CUFT                  1256.9
PRESSURE DROP OPTION:                                      SPECIFIED

HOLDUP OPTION:                                             NO-SLIP

ERROR TOLERANCE                                            0.10000E-03
INTEGRATION METHOD                                         GEAR
CORRECTOR METHOD                                           NEWTON
INITIAL STEP SIZE FACTOR                                   0.10000E-01
CORRECTOR TOLERANCE FACTOR                                 0.10000
MAXIMUM NUMBER OF STEPS                                     1000

TEMPERATURE PROFILES:

  RELATIVE LOCATION          TEMPERATURE
       0.0000                530.00        F


                       ***  RESULTS  ***

 REACTOR DUTY BTU/HR  0.26453E+08
 RESIDENCE TIME HR  0.98390E-02
 REACTOR MINIMUM TEMPERATURE F  530.00
 REACTOR MAXIMUM TEMPERATURE F  530.00

        *** RESULTS PROFILE (PROCESS STREAM) ***


    LENGTH        PRESSURE      TEMPERATURE    VAPOR FRAC    RES-TIME
    FT            PSIA          F                            HR

     0.0000        88.176        530.00       0.98724        0.0000
     13.232        88.176        530.00       0.95776       0.99148E-03
     26.463        88.176        530.00       0.95684       0.19765E-02
     39.695        88.176        530.00       0.95651       0.29603E-02
     52.927        88.176        530.00       0.95634       0.39435E-02
     66.158        88.176        530.00       0.95623       0.49264E-02
     79.390        88.176        530.00       0.95616       0.59091E-02
     92.621        88.176        530.00       0.95611       0.68917E-02
     105.85        88.176        530.00       0.95607       0.78742E-02
     119.08        88.176        530.00       0.95604       0.88566E-02
     132.32        88.176        530.00       0.95601       0.98390E-02

    LENGTH        DUTY          LIQUID HOLDUP
    FT            BTU/HR
     0.0000        0.0000       0.23517E-03
     13.232       0.26134E+07   0.14095E-02
     26.463       0.27905E+07   0.14574E-02
     39.695       0.28534E+07   0.14743E-02
     52.927       0.28849E+07   0.14829E-02
     66.158       0.29034E+07   0.14881E-02
     79.390       0.29151E+07   0.14914E-02
     92.621       0.29229E+07   0.14938E-02
```

```
     105.85        0.29283E+07   0.14956E-02
     119.08        0.29321E+07   0.14969E-02
     132.32        0.29349E+07   0.14980E-02


        *** TOTAL MOLE FRACTION PROFILE (PROCESS STREAM) ***

    LENGTH HDMA ADA WATER NYLON-66 FT
```

```
 0.0000       0.42140E-01  0.41791E-01  0.91594       0.0000
 13.232       0.53305E-02  0.22422E-02  0.95511      0.37193E-01
 26.463       0.28718E-02  0.92728E-03  0.95730      0.38782E-01
 39.695       0.19697E-02  0.49386E-03  0.95808      0.39337E-01
 52.927       0.14982E-02  0.28496E-03  0.95848      0.39619E-01
 66.158       0.12074E-02  0.16976E-03  0.95872      0.39785E-01
 79.390       0.10101E-02  0.10324E-03  0.95887      0.39893E-01
 92.621       0.86730E-03  0.64420E-04  0.95898      0.39966E-01
 105.85       0.75931E-03  0.41849E-04  0.95906      0.40017E-01
 119.08       0.67482E-03  0.28775E-04  0.95912      0.40056E-01
 132.32       0.60698E-03  0.21163E-04  0.95917      0.40086E-01

LENGTH N2O FT


 0.0000       0.12501E-03
 13.232       0.12077E-03
 26.463       0.12041E-03
 39.695       0.12028E-03
 52.927       0.12021E-03
 66.158       0.12017E-03
 79.390       0.12015E-03
 92.621       0.12013E-03
 105.85       0.12012E-03
 119.08       0.12011E-03
 132.32       0.12010E-03

    *** TOTAL MASS FRACTION PROFILE (PROCESS STREAM) ***

LENGTH HDMA ADA WATER NYLON-66 FT


 0.0000       0.17800      0.22200      0.59980       0.0000
 13.232       0.23308E-01  0.12330E-01  0.64744      0.31673
 26.463       0.12594E-01  0.51143E-02  0.65085      0.33124
 39.695       0.86474E-02  0.27267E-02  0.65208      0.33634
 52.927       0.65811E-02  0.15742E-02  0.65271      0.33894
 66.158       0.53056E-02  0.93811E-03  0.65308      0.34047
 79.390       0.44392E-02  0.57065E-03  0.65333      0.34146
 92.621       0.38123E-02  0.35612E-03  0.65350      0.34214
 105.85       0.33380E-02  0.23137E-03  0.65362      0.34261
 119.08       0.29668E-02  0.15910E-03  0.65370      0.34297
 132.32       0.26687E-02  0.11702E-03  0.65377      0.34324

LENGTH N2O FT

 0.0000       0.20000E-03
 13.232       0.20000E-03
 26.463       0.20000E-03
 39.695       0.20000E-03
 52.927       0.20000E-03




                              ~APD07C.tmp
 66.158       0.20000E-03
 79.390       0.20000E-03
 92.621       0.20000E-03
 105.85       0.20000E-03
 119.08       0.20000E-03
 132.32       0.20000E-03
```

```
    *** LIQUID MOLE FRACTION PROFILE (PROCESS STREAM) ***

 LENGTH HDMA ADA WATER NYLON-66 FT


  0.0000        0.47544E-01   0.84262        0.10983        0.0000
  13.232        0.46408E-02   0.25272E-01   0.89493E-01   0.88059
  26.463        0.24695E-02   0.10281E-01   0.88590E-01   0.89866
  39.695        0.16864E-02   0.54437E-02   0.88279E-01   0.90459
  52.927        0.12801E-02   0.31318E-02   0.88131E-01   0.90745
  66.158        0.10304E-02   0.18625E-02   0.88048E-01   0.90906
  79.390        0.86131E-03   0.11314E-02   0.87997E-01   0.91001
  92.621        0.73921E-03   0.70537E-03   0.87964E-01   0.91059
  105.85        0.64695E-03   0.45796E-03   0.87943E-01   0.91095
  119.08        0.57485E-03   0.31475E-03   0.87930E-01   0.91118
  132.32        0.51699E-03   0.23141E-03   0.87923E-01   0.91133

 LENGTH N2O FT


  0.0000        0.32689E-05
  13.232        0.24685E-05
  26.463        0.24307E-05
  39.695        0.24176E-05
  52.927        0.24112E-05
  66.158        0.24075E-05
  79.390        0.24052E-05
  92.621        0.24037E-05
  105.85        0.24027E-05
  119.08        0.24020E-05
  132.32        0.24016E-05


    *** LIQUID MASS FRACTION PROFILE (PROCESS STREAM) ***

 LENGTH HDMA ADA WATER NYLON-66 FT


  0.0000        0.42289E-01   0.94256        0.15145E-01    0.0000
  13.232        0.26289E-02   0.18004E-01   0.78592E-02   0.97151
  26.463        0.13879E-02   0.72664E-02   0.77187E-02   0.98363
  39.695        0.94532E-03   0.38376E-02   0.76715E-02   0.98755
  52.927        0.71663E-03   0.22050E-02   0.76490E-02   0.98943
  66.158        0.57645E-03   0.13104E-02   0.76365E-02   0.99048
  79.390        0.48166E-03   0.79568E-03   0.76288E-02   0.99109
  92.621        0.41327E-03   0.49594E-03   0.76240E-02   0.99147
  105.85        0.36163E-03   0.32194E-03   0.76209E-02   0.99170
  119.08        0.32129E-03   0.22124E-03   0.76190E-02   0.99184
  132.32        0.28893E-03   0.16265E-03   0.76178E-02   0.99193
LENGTH N2O FT

 0.0000  0.11013E-05
 13.232  0.52963E-06
```

```
  26.463        0.51741E-06
  39.695        0.51327E-06
  52.927        0.51127E-06
  66.158        0.51013E-06
  79.390        0.50943E-06
  92.621        0.50898E-06
```

```
 105.85        0.50868E-06
 119.08        0.50848E-06
 132.32        0.50835E-06

    *** VAPOR MOLE FRACTION PROFILE (PROCESS STREAM) ***

LENGTH HDMA ADA WATER NYLON-66 FT


 0.0000        0.42070E-01   0.31439E-01   0.92636        0.0000
 13.232        0.53609E-02   0.12266E-02   0.99329        0.75264E-80
 26.463        0.28900E-02   0.50542E-03   0.99648        0.39040E-80
 39.695        0.19826E-02   0.26883E-03   0.99762        0.22341E-80
 52.927        0.15082E-02   0.15500E-03   0.99821        0.14214E-80
 66.158        0.12155E-02   0.92289E-04   0.99857        0.98450E-81
 79.390        0.10169E-02   0.56106E-04   0.99880        0.72835E-81
 92.621        0.87318E-03   0.34998E-04   0.99897        0.56873E-81
 105.85        0.76447E-03   0.22730E-04   0.99909        0.46571E-81
 119.08        0.67942E-03   0.15626E-04   0.99918        0.39794E-81
 132.32        0.61113E-03   0.11490E-04   0.99925        0.35297E-81

LENGTH N2O FT


 0.0000        0.12659E-03
 13.232        0.12598E-03
 26.463        0.12573E-03
 39.695        0.12564E-03
 52.927        0.12559E-03
 66.158        0.12556E-03
 79.390        0.12555E-03
 92.621        0.12554E-03
 105.85        0.12553E-03
 119.08        0.12552E-03
 132.32        0.12552E-03

    *** VAPOR MASS FRACTION PROFILE (PROCESS STREAM) ***

LENGTH HDMA ADA WATER NYLON-66 FT


 0.0000       0.18675        0.17552       0.63752        0.0000
 13.232       0.33310E-01    0.95847E-02   0.95681        0.91078E-79
 26.463       0.18284E-01    0.40215E-02   0.97739        0.48106E-79
 39.695       0.12625E-01    0.21530E-02   0.98492        0.27709E-79
 52.927       0.96368E-02    0.12455E-02   0.98881        0.17689E-79
 66.158       0.77827E-02    0.74312E-03   0.99117        0.12276E-79
 79.390       0.65194E-02    0.45237E-03   0.99272        0.90943E-80
 92.621       0.56033E-02    0.28244E-03   0.99381        0.71079E-80
 105.85       0.49090E-02    0.18356E-03   0.99460        0.58243E-80
 119.08       0.43651E-02    0.12625E-03   0.99520        0.49792E-80
 132.32       0.39279E-02    0.92873E-04   0.99567        0.44184E-80
LENGTH N2O FT



                             ~APD07C.tmp
 0.0000        0.21283E-03

 13.232        0.29649E-03
 26.463        0.30129E-03
 39.695        0.30303E-03
 52.927        0.30394E-03
```

```
 66.158        0.30449E-03
 79.390        0.30486E-03
 92.621        0.30511E-03
 105.85        0.30530E-03
 119.08        0.30544E-03
 132.32        0.30556E-03

    *** COMPONENT ATTRIBUTE PROFILE (PROCESS SUBSTREAM ) ***

LENGTH          NYLON-66       NYLON-66       NYLON-66       NYLON-66
FT              SFRAC          SFRAC          SFRAC          SFRAC
                HDMA-E         ADA-E          HDMA-R         ADA-R

 0.0000          0.0000         0.0000         0.0000         0.0000
 13.232         0.65527E-02    0.81400E-01    0.47474        0.43731
 26.463         0.45204E-02    0.46268E-01    0.48504        0.46417
 39.695         0.42689E-02    0.33386E-01    0.48845        0.47389
 52.927         0.44663E-02    0.26700E-01    0.48998        0.47886
 66.158         0.48332E-02    0.22535E-01    0.49074        0.48189
 79.390         0.52751E-02    0.19634E-01    0.49114        0.48396
 92.621         0.57490E-02    0.17471E-01    0.49132        0.48546
 105.85         0.62312E-02    0.15796E-01    0.49138        0.48659
 119.08         0.67055E-02    0.14474E-01    0.49135        0.48747
 132.32         0.71611E-02    0.13417E-01    0.49127        0.48815

LENGTH          NYLON-66       NYLON-66       NYLON-66       NYLON-66
FT              SFLOW          SFLOW          SFLOW          SFLOW
                HDMA-E         ADA-E          HDMA-R         ADA-R

 0.0000          0.0000         0.0000         0.0000         0.0000
 13.232         0.67985E-04    0.84454E-03    0.49254E-02    0.45372E-02
 26.463         0.49300E-04    0.50460E-03    0.52899E-02    0.50623E-02
 39.695         0.47363E-04    0.37041E-03    0.54193E-02    0.52578E-02
 52.927         0.49983E-04    0.29880E-03    0.54834E-02    0.53590E-02
 66.158         0.54366E-04    0.25349E-03    0.55202E-02    0.54206E-02
 79.390         0.59535E-04    0.22159E-03    0.55429E-02    0.54619E-02
 92.621         0.65031E-04    0.19763E-03    0.55577E-02    0.54914E-02
 105.85         0.70601E-04    0.17898E-03    0.55674E-02    0.55132E-02
 119.08         0.76068E-04    0.16419E-03    0.55739E-02    0.55299E-02
 132.32         0.81313E-04    0.15235E-03    0.55783E-02    0.55428E-02

LENGTH          NYLON-66       NYLON-66       NYLON-66       NYLON-66
FT              EFRAC          EFRAC          ZMOM           FMOM
                HDMA-E         ADA-E          ZMOM           FMOM

 0.0000          0.0000         0.0000         0.0000         0.0000
 13.232         0.74503E-01     0.92550       0.45626E-03    0.10375E-01
 26.463         0.89005E-01     0.91100       0.27695E-03    0.10906E-01
 39.695         0.11337         0.88663       0.20889E-03    0.11095E-01
 52.927         0.14331         0.85669       0.17439E-03    0.11191E-01
 66.158         0.17660         0.82340       0.15393E-03    0.11249E-01
 79.390         0.21178         0.78822       0.14056E-03    0.11286E-01
 92.621         0.24759         0.75241       0.13133E-03    0.11312E-01
 105.85         0.28288         0.71712       0.12479E-03    0.11330E-01
 119.08         0.31661         0.68339       0.12013E-03    0.11344E-01
 132.32         0.34799         0.65201       0.11683E-03    0.11355E-01
```

```
                        ~APD07C.tm
                             p


LENGTH          NYLON-66        NYLON-66
FT              DPN             MWN
                DPN             MWN

 0.0000           0.0000          0.0000
 13.232           22.739          2603.9
 26.463           39.379          4486.4
 39.695           53.114          6040.0
 52.927           64.173          7290.4
 66.158           73.077          8297.1
 79.390           80.292          9112.4
 92.621           86.133          9772.4
 105.85           90.796          10299.
 119.08           94.432          10709.
 132.32           97.190          11021.
```

Aspen HYSYS Screenshots

Pump and Heat Exchanger Sizing

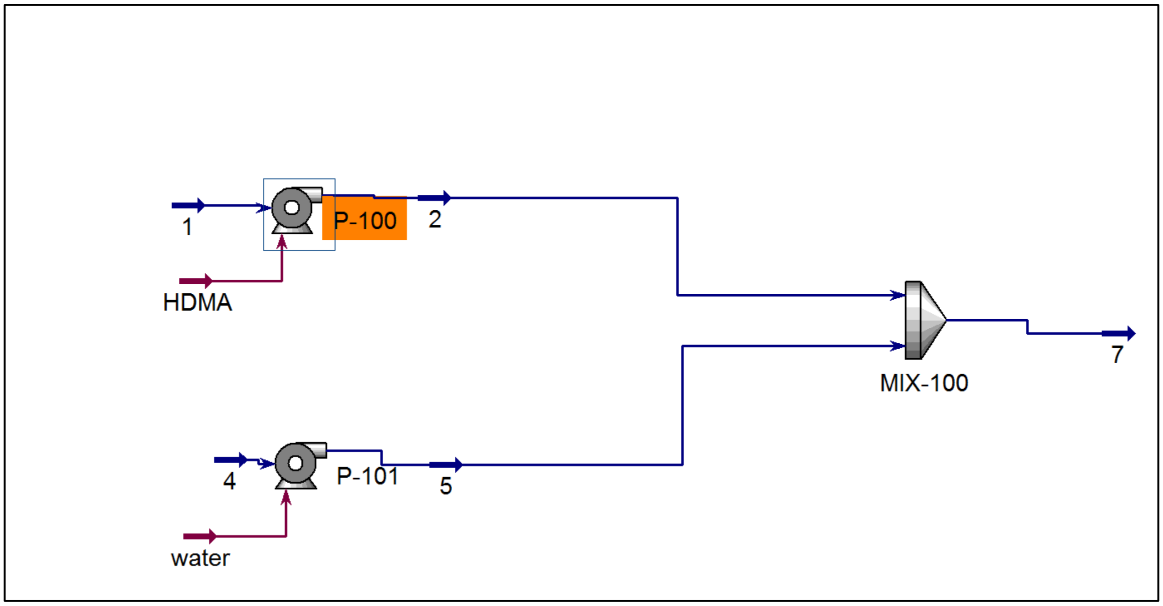


Figure A13. Aspen HYSYS Simulation Flowsheet for Pump Sizing

Pre-Feed Heater Simulation

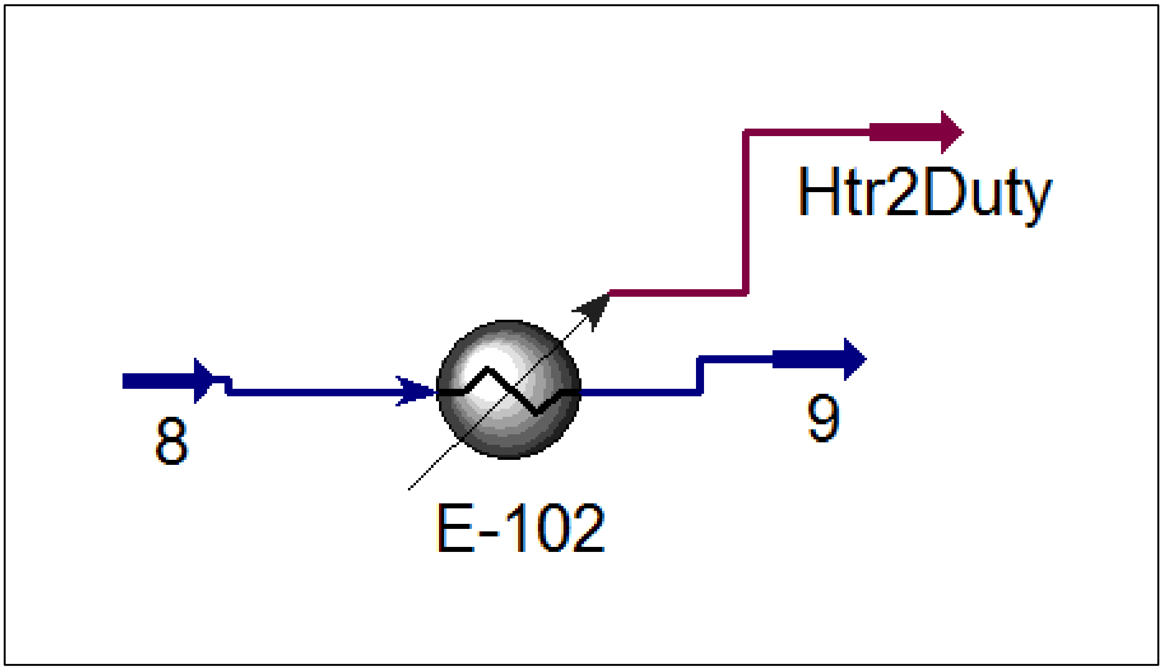


Figure A14. Aspen HYSYS Simulation Flowsheet for Pre-Feed Heater Simulation

Salt Heater and Pump Simulation

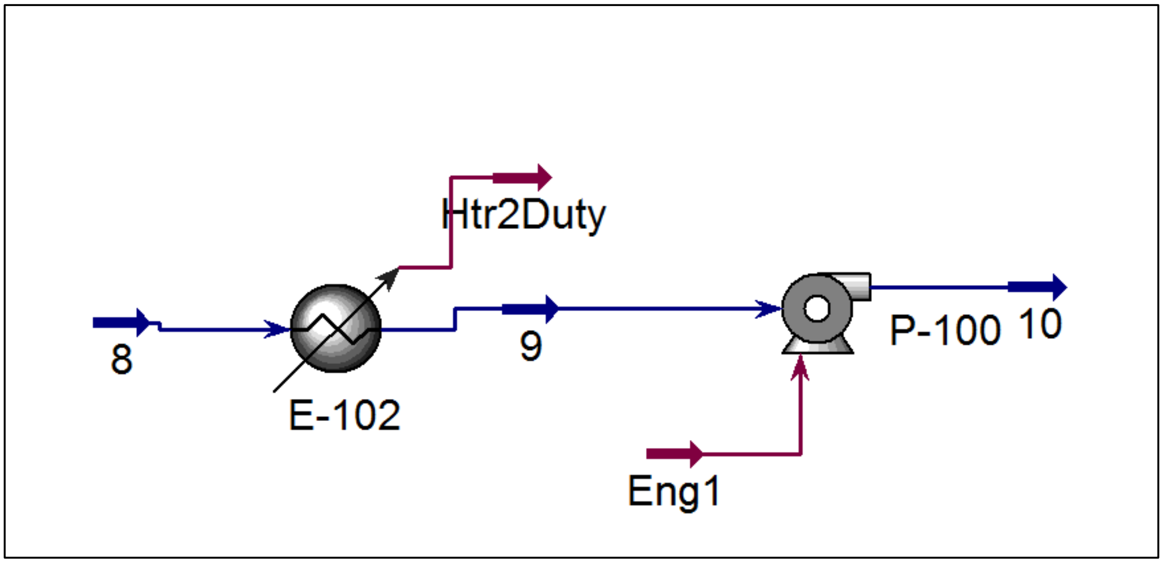


Figure A15. Aspen HYSYS Simulation Flowsheet for Salt Heater and Pump Simulation

Mixer Sizing and Low NOx Burner Sizing

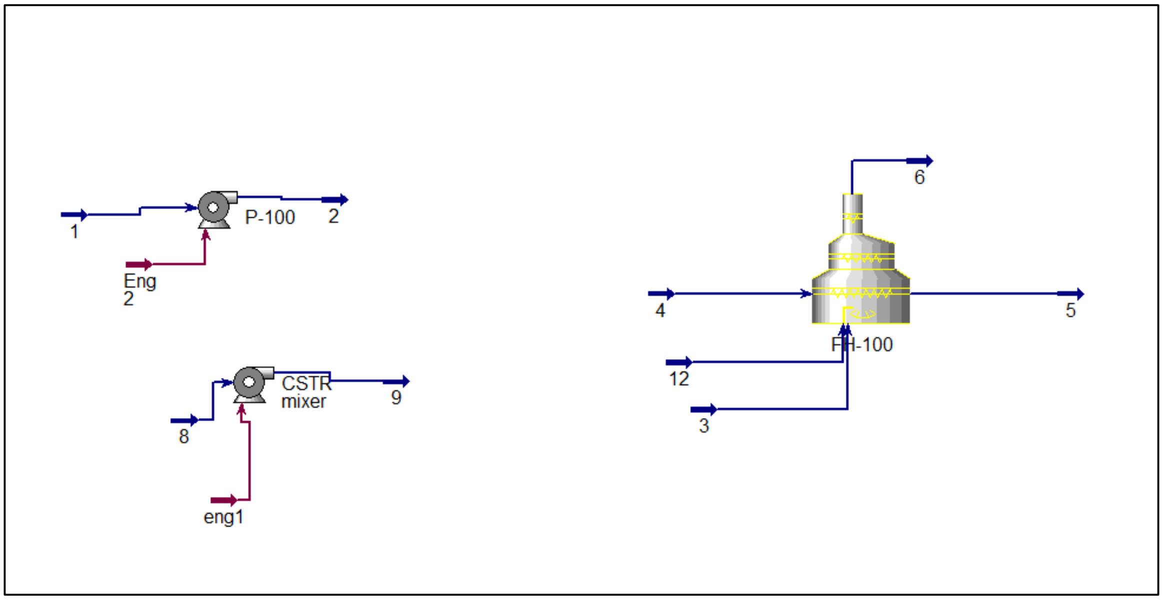


Figure A16. Aspen HYSYS Simulation Flowsheet for Mixer Sizing and NOx Burner Sizing