University of Arkansas, Fayetteville

ScholarWorks@UARK

Chemical Engineering Undergraduate Honors Theses

Chemical Engineering

5-2017

An industrial process for the production of nylon 6 6 through the step-growth reaction of adipic acid and hexamethylenediamine

David Wallace Jacobson University of Arkansas, Fayetteville

Follow this and additional works at: https://scholarworks.uark.edu/cheguht

Part of the Polymer Science Commons

Citation

Jacobson, D. W. (2017). An industrial process for the production of nylon 6 6 through the step-growth reaction of adipic acid and hexamethylenediamine. *Chemical Engineering Undergraduate Honors Theses* Retrieved from https://scholarworks.uark.edu/cheguht/104

This Thesis is brought to you for free and open access by the Chemical Engineering at ScholarWorks@UARK. It has been accepted for inclusion in Chemical Engineering Undergraduate Honors Theses by an authorized administrator of ScholarWorks@UARK. For more information, please contact scholar@uark.edu, uarepos@uark.edu.

An industrial process for the production of nylon 6 6 through the step-growth reaction of adipic acid and hexamethylenediamine

Authors: David Jacobson, University of Arkansas Department of Chemical Engineering

Date of Submittal: 3/3/2017

Contents

Section 1: Letter of Transmittal*
Section 2: Title Page1
Section 3: Table of Contents
Section 4: Abstract
Section 5: Introduction
Section 6: Material Balances and Process Flow Diagram6
Section 7: Process Description9
Section 8: Energy Balance and Utility Requirements11
Section 9: Equipment List and Unit Descriptions12
Section 10: Equipment Specification Sheets15
Section 11: Equipment Cost Summary25
Section 12: Fixed Capital Investment Summary26
Section 13: Safety, Health, and Environmental Considerations27
Section 14: Other Important Considerations
Section 15: Manufacturing Costs
Section 16: Economic Analysis
Section 17: Conclusions and Recommendations
Section 18: Acknowledgements
Section 19: Bibliograph
Section 20: Appendix

Section 4: Abstract

A continuous, two stage, four reactor system process is presented here for the proposed purpose of nylon 6 6 manufacture at the rate of 85 million lbs per year. Report components include: process descriptions, simulation methods and results, economic analysis, EH&S considerations, process control descriptions, and a general recommendation for how to proceed with plans enclosed. The general design of the plant is a two stage system composed of one PFR used for the formation of nylon salt and low molecular weight nylon chains, followed by three CSTR's used for increasing nylon molecular weight. The overall process has been found to be profitable and exceeds the typical hurdle rate associated with textile production (~30%). This being said, there are considerable EH&S considerations associated with the process itself as well as the implications associated with operating a plant in Calvert City Kentucky that will need to receive due attention before a decision is made on whether to build said plant.

Attributes unique to this plant include its solid feed handling system that allows the plant to use water generated solely by the polymerization reaction, during steady state operation. Additionally, the three CSTR reactors used for driving up polymer molecular weight provide exceptional process adaptability that allows for such plants to remain profitable even during economic down turns and severe market fluctuations.

Section 5: Introduction

The following report outlines a chemical process and related considerations for the production of nylon 6 6 in Calvert City Kentucky. The process consists of a two stage four reactor system capable of producing in excess of 85 million lbs of nylon per year. The first reactor stage is responsible for the initial reaction of nylon salt (adipic acid and HMDA in aqueous solution) to form low molecular weight nylon. A flash drum is then utilized to remove water from the reactor 1 exit stream. This allows for continued nylon chain growth that takes place in three parallel CSTRs. The resulting molten nylon is then fed to an extruder where it is solidified and granulated.

The nylon 6 6 manufacturing process is well reported in the literature (Source 1-6). Components of this plant that are unique and give it an economic advantage over traditional designs include the economic versatility that results from the use of three rather than one CSTR during the second reaction stage, as well as the dry feed handling system that allows for efficient water use. It is generally considered better to use one large reactor rather than multiple smaller reactors in parallel in order to take advantage of the economies of scale and reduce the fixed capital investment associated with a project. For this process though, utilizing three parallel reactors is highly advantageous in that it allows for the simultaneous production of nylon product streams with different molecular weights. The molecular weight of nylon is a function of the CSTR residence time, thus differing weights of nylon could be produced by altering the feed rate to each reactor. The molecular weight of nylon determines its properties, potential uses, and price. Being able to produce different molecular weights of nylon simultaneously allows for access to a larger product market as well as the ability to maximize profits by altering production to take advantage of fluctuations in market demand and prices. Additionally, having three CSTR's makes it much easier to bring the plant down to 67% production capacity by simply reducing the feed rate and closing the valve to one reactor.

Also notable in this plant is its efficient use of water. By employing a high recycle rate and a solid feed melting system, the process can be operated solely using the water generated by the polymerization reaction. Dry HDMA is fed to a process tank where it is melted using heat from the recycle stream before being pressurized and further heated to reactor conditions. Adipic acid cannot be introduced to the process as a pure liquid, and as a result is mixed with condensed recycled steam before being pressurized, heated, and mixed with the HDMA. This system not only eliminates the need for feed water, but also significantly decreases energy costs, safety costs, and costs associated with chemical storage. Storing HDMA and adipic acid in dilute solution would require much larger storage systems as well as additional equipment and energy to flash off the excess water in order to concentrate reactants. Furthermore aqueous HDMA is corrosive, posing a hazard to vessel integrity during storage. Dry chemical storage avoids this problem entirely.

Extensive economic analysis was performed to ensure that this process will be profitable. The grass roots method was used for determining the fixed capital investment (FCI) while the COM method was used for calculating manufacturing costs (Source 7, pg205). The results of these analyses can be found in sections 12, 13, and 16. The internal rate of return was found to be 54.5%, far over the standard hurdle rate for bulk chemicals (usually 20-30%). This indicates that the process is likely to be highly lucrative, although it is the author's opinion that the FCI is underestimated.

Environmental, healthy, and safety (EH&S) considerations are provided in section 13. Significant hazards exist within the process that are associated with: the flammability, toxicity, and volatility of the materials used; high operating pressures; and high operating temperatures. HMDA and adipic acid are both flammable and toxic. In the dry form, both of these chemicals can form explosive air dust mixtures. A dust collector, ventilation system, specialized processing equipment, and personal protection equipment such as respirators will need to be utilized to minimize the risks associated with the solid and liquid handling of these chemicals. Much of the process is ran at high temperature and pressures in

order to ensure proper stoichiometric ratios of reactants as well as optimal conditions for reaction to take place. Pressure relief devices, temperature control equipment, a sophisticated process control system, and regular safety inspection of equipment will be needed to properly regulate this process and ensure its operation in a safe manner.

Section 6: Material Balances and Process flow diagram

	lb/year	lb/hr
nylon 66 production rate	86700000	10997
adipic acid	56488120.59	7165
hexamethylene diamine	44917761.61	5697

Figure (6.1): Calculated Mass Balance – Material Requirements

Figure 6.2: Simulated Mass Balance

Simulator Mass Balance						
Streams	mass flow rate (lb/hr)	in / out				
LIQHDMA	5555.649	IN				
ADA	7098.885	IN				
P3A	3646.375	OUT				
P3B	3646.419	OUT				
P3C	3646.342	OUT				
WASTE H2O	1715.144	OUT				
NET	-0.254					

Description:

Figure 6.1 provides the mass flow rates necessary to produce 85 million lbs of nylon per year. These values are assuming that the plant (up time) is 90% and that the production goal will be exceeded by 2%. Figure 6.2 provides the mass flows associated with the process simulation. One can see that a net 0.254 lbs are lost during the simulator, but this value is small enough to be attributed to round off errors by the simulator and does not reflect a faulty process.

Figure 6.3: Process Flow Diagram



Figure 6.4: Feed System Diagram



Section 7: Process Description

The nylon production process presented here utilizes a two stage 4 reactor system for the production of approximately 85 million lbs / year of nylon 6 6. The first stage of production is observed in figure 6.4, where a hopper system is used to feed solid Hexamethylenediamine (HMDA) to a heated vessel where it is melted and further heated to 325K. Melting the (HMDA) allows for it to be introduced to the process without (water), allowing for lower (recycle rates) and smaller vessel sizes. Adipic acid (ADA) cannot be melted while pure due to its high melting point and associated explosion hazards. To address these issues, ADA is fed through an identical hopper system to a heated vessel filled with boiling water where it can fully dissolve. Solubility calculations can be found in Appendix A1. Neither of these feed systems were not included in the simulation due to issues with modelling the correct thermodynamics associated with solid liquid equilibrium during the melting of HMDA and the dissolution of ADA.

Both feed streams are pressurized from 1 to 10 atm, and heated to 450K before being mixed and fed to reactor 1. Increasing the temperature and pressure of each stream ensures that the two streams are completely soluble during mixing to form a nylon salt solution. Additionally, the first stage of polymerization will only occur at high temperatures. Pressurization ensures that water and HDMA remain in the liquid phase during the reaction.

Reactor 1 (R1) facilitates the first stage of the polymerization reaction where the nylon salt solution reacts to form short nylon chains. A 50m long plug flow reactor with a diameter varying from 0.45m to 0.6m across its length is employed to facilitate this reaction. The degree of polymerization across the reactor length is shown in Figure 7.1. As polymerization occurs, the viscosity of the nylon solution will increase across the length of the reactor. The widening reactor diameter is used to decrease the pressure drop across the reactor. The reactor is heated from 450K to 555K across the length of the reactor as a result of the exothermic chemical reaction as well as a counter current flow of high temperature steam. Increasing the reactor temperature drives the reaction forward to produce higher molecular weight nylon, as well as to decrease fluid viscosity and ensure that nylon formed does not solidify prematurely.



Figure 7.1: DPN vs PFR length

The nylon solution from reactor 1 is fed to a heated flash drum (FLASH 1) where it is flashed at 600K and 1atm. The resulting liquid stream is rich in low molecular weight nylon with trace concentrations of ADA and HDMA, and is fed to the three CSTR reactors (R2A, R2B, R2C). The flashing process removes most of the water from the liquid nylon, resulting in additional reactions to form higher molecular weight nylon. The resulting vapor stream is rich in water with trace concentrations of ADA and HDMA, and is fed to the recycle and waste water streams.

The three CSTR reactors provide sufficient time for nylon to continue to react to achieve higher molecular weights. Three CSTR's were included in the design so that nylon streams with differing molecular weights could be manufactured simultaneously by controlling the flow rate to each reactor and by extension the residence time. This will increase the capitol cost associated with the plant, but provides versatility that could prove extremely useful for ensuring steady profits. For example if low molecular weight nylon demand dropped, the overall production rate and flow rates to each reactor could be altered so that low molecular weight nylon could be produced in two of the reactors for existing customers while the third reactor could be used for the manufacture of more lucrative high molecular weight nylon. This ability to adapt to and ride out oscillations in economic markets is highly useful and reduces investment risks. Having three reactors also allows the process to be easily changed from 100% capacity to 67% capacity by simply shutting off flows to one of the reactors and reducing the feed rate.

Nylon exiting the CSTR's will be fed to an extruder and granulated before being packaged for transport and sale. The extruding process cannot be modelled in aspen and is not included in the process flow diagram. The vent stream from each reactor will be mixed with the vapor stream from the flash drum before being used to heat the ADA-water feed stream (PRES-ADA), the liquefied HDMA stream (PRESHDMA), and the HDMA melting vessel (heater 2). The steam is condensed during the melting of HDMA, and is fed through a splitter where (25%) exits the process for waste treatment, and 75% is mixed with the incoming solid ADA stream.

Section 8: Energy Balance and Utility Requirements

	U		/			
	LIQHDMA	ADA	P3A	P3B	P3C	WASTEH2O
FLOW RATE (Kg/hr)	2520	3220	1653.96	4653.99	4653.95	776.871
TEMP (K)	325	373	600	600	600	370
PRESSURE (atm)	1	1	1	1	1	10
ENTHALPY (KJ/kg)	-1240	-6480	-998.19	-1001.1	-1001.1	-15549
ENERGY FLOWS (KJ/hr)	-3124800	-2.1E+07	-1650966	-4659109	-4659069	-12079567.18

Figure 8.1: Entering and Exiting Process Stream Thermodynamic Data

Figure 8.2: Non-stream Energy Sources

	HEAT1	HEAT2	HEAT3	PUMP1	PUMP2	FLASH2	plug	total
heat/energy duty (kW)	0	-1932	176.88	2.28	4.26	282.681	3398	1932
heat/energy duty (kj/hr)	0	-7E+06	636761	8208	15336	1017652	1E+07	7E+06
energy source	E	NG	NG	E	E	NG	NG	
corrected heat duty (kW)	0	-3864	353.76	2.28	4.26	565.362	6796	

Legend (E= electricity, NG= natural gas / boiler system)

Figure 8.3: Overall Simulation Energy Balance

Enthalpy IN (Kj/hr)	-2.4E+07
Enthalpy OUT (Kj/hr)	-2.3E+07
Net energy summary (Kj/hr)	6955196
Net energy input	-7896884

Figure 8.4: Overall utility requirements

Utility Costs	\$/Kwh	yearly energy demand (Kwh)	yearly cost (\$)
Electricity	0.0535*	51561.36	2758.53276
Natural Gas	0.0127**	30360637.51	385580.0964
Total Utility			388338.6292

*Bibliography source 9

**Bibliography source 10

Section 9: Equipment List and Unit Descriptions

Figure 9.1: Thermal Equipment Attributes

	HEAT1 (startup only)	HEAT2 (FEED HEATING) X2	HEAT3	HX1	hx2	BOILER
Aspen Capacity (m2)	Х	10	х	1.4	16.37	x
Actual Capacity (m2)	Х	12	х	1.68	19.644	x
PRESSURE (atm)	Х	1	х	10	10	х
PRESSURE (barg)	Х	1.0125	Х	9.11925	9.11925	х
heat duty (kW)	0	-1408.5	172.9	214.8	188.161	3779.34
stream comp cold	Х	H2O+ADA	х	h2O+ADA	HMDA	H2O
stream comp hot	Х	H2O	Х	H2O	H2O	H2O
Material	CS	CS	SS	SS-TUBE, CS-SHELL	CS	x
ТҮРЕ	Electric	hx-redirect	hx-boiler fired	shell and tube	counter current tube bank	BOILER
MATERIAL FACTOR	Х	1.8	х	1.8	1	Х
PRESSURE FACTOR	X	1	х	1.01393826 5	1.013938265	x
c1	Х	0.03881	х	0.03881	0.03881	Х
c2	Х	-0.11272	Х	-0.11272	-0.11272	Х
c3	Х	0.08183	Х	0.08183	0.08183	Х
B1	Х	1.74	Х	1.74	1.74	Х
B2	Х	1.55	Х	1.55	1.55	Х
CP0(2001)	Х	9120	Х	2016	7366.5	510210.9
CEPCI (2001)	397	397	397	397	397	397
CEPCI (2016)	556.8	556.8	556.8	556.8	556.8	556.8
COST	10000	57943.1044 8	12918.4300 2	12918.4300 2	34214.35462	715580.42 6
METHOD	INTERNET SOURCE	HX2 BASIS	HX1 BASIS	BMC	BMC	Capcost- BMC

Figure 9.2: Reactor and Proc	cess Vessel Attributes
------------------------------	------------------------

			FLASH				
	CSTR(X3)	PFR	DRUM	FEED vessel (x2)			
CAPACITY (m3)	10	11	1	0.2			
Operating temp (k)	600	500	600	325K			
Operating press							
(atm)	1	10	5.5	1			
Operating press							
(barg)	0	9.11925	4.559625	0			
diameter(m)	1.5	0.525		0.3			
Length (m)	5.658842421	50		2.829421211			
MATERIAL	CS	SS (CLAD)	CS	CS			
MATERIAL FACTOR	1	1.7	1	1			
PRESSURE FACTOR	1	1	1	1			
c1	x	x	x	x			
c2	x	x	x	x			
c3	x	x	x	x			
B1	1.49	1.49	1.49	1.49			
B2	1.52	1.52	1.52	1.52			
CP0(2001)	72000	192500	19500	4000			
CEPCI (2001)	397	397	397	397			
CEPCI (2016)	556.8	556.8	556.8	556.8			
COST	303953.8942	1099918.428	82320.84635	16886.32746			
METHOD	BMC	BMC	BMC	ВМС			
NOTES		averages used	d for vars that v	averages used for vars that varied with length			

Figure 9.3: Flow Equipment Attributes

	MIXER(x3)	PUMP1	PUMP2	splitter (x2)
volumetric flow rate (m3/s)	х	0.000835	0.001558073	х
pressure change (Pa)	х	911250	911250	х
Ideal Power (Kw)	х	0.76089375	1.419794325	х
Power (Kw)	х	2.284966216	4.263646622	х
STREAM COMP	х	HMDA	ADA+H2O	х
MATERIAL	x	CS	SS	х
MATERIAL FACTOR	х	1.55	2.3	х
PRESSURE FACTOR	х	1	1	х
c1	x	0	0	x
c2	x	0	0	x
c3	х	0	0	х
B1	x	1.89	1.89	x
B2	x	1.35	1.35	x
CP0(2001)	х	2741.959459	3197.734966	х
CEPCI (2001)	x	397	397	x
CEPCI (2016)	х	556.8	556.8	х
COST	0	15315.30089	22401.99409	0
Method	x	BMC	BMC	x
NOTES	PG365			PG365

Figure 9.4: Specialty Equipment Attributes

	dust collector	hopper (x2)	extruder
Volume	30	x	x
CP0(2001)	30000	x	x
CEPCI (2001)	397	x	x
CEPCI (2016)	556.8	x	x
COST	42083.12343	3000	42000
METHOD	BMC	Internet Source (13)	Internet Source (12)

Section 10: Equipment Specification Sheets

	PUMP 1					
Identification:	Item	Centrifugal Pump				
	No. required	1		Date: 2 March 2017		
				By: David Jacobson		
Function: Pres	surize liquid HDI	MA from 1 to 10 atm				
Operation: Co	ntinuous					
Materials hand	lled	LIQHDMA	HOTHDMA			
Quantity (I	b/hr)	5556	5556			
Compositio	on					
HDMA		1	1			
Temperature (К):	325	325			
Design Data:	Operating pres	sure: 10atm				
	Material: Carb	on Steel				
	Flow Rate:					
	Impellar size:					
Efficiency:						
	Power: 2.29 k\	V				
Utilities:	electrical pow	er				
Controls:						
Tolerances:						

PUMP 2						
Identification: Item	Centrifugal Pump					
No. requ	ired 1		Date: 2 March 2017			
			By: David Jacobson			
Function: Pressurize H2C	Function: Pressurize H2O-Adipic Acid solution from 1 to 10 atm					
Operation : Continuous						
Materials handled	ADAH2O	PRES-ADA				
Quantity (lb/hr)	1244.1	12244.1				
Composition (lb/hr)						
HDMA	1.144	1.144				
ADA	7101.76	7101.76				
H2O	5141.6	5141.6				
NYLON66	TRACE	TRACE				
Temperature (K):	372	372				
Design Data: Operatin	g pressure: 10atm					
Material	: Stainless Steel					
Flow Rat	e: 106.2 ft3/hr					
Impellar	size:					
Efficienc	y:					
Power: 4	.2636 kW					
Utilities: electrica	al power					
Controls:						
Tolerances:						

	Mixer1					
Identification: Item	Piping Tee					
No. requi	red 1		Date: 2 March 2017			
			By: David Jacobson			
Function: Facilitate the m	ixing of ADA with water					
Operation: Continuous						
Materials handled	ADA	COND-H2O	ADA-H2O			
Quantity (lb/hr)	7098.89	2333.814	5553.81			
Composition (lb/hr)						
HDMA	0	1.144	1.144			
ADA	7098.89	2.87442	7101.76			
H2O	0	5141.6	5141.6			
NYLON66	0	TRACE	TRACE			
Temperature (K):	373	373	373			
Design Data: Operating	g pressure: 1atm					
Material:	Stainless Steel					
Flow Rate	e: 198.1 ft3/hr					
Utilities:						
Controls:						
Tolerances:						

Mixer2					
Identification: Item	Piping Tee				
No. requ	ired 1		Date: 2 March 2017		
			By: David Jacobson		
Function: Facilitate the n	nixing of the ADA-water so	olution with HDMA			
Operation: Continuous					
Materials handled	FEEDADA	FEEDHDMA	MIX-1		
Quantity (lb/hr)	12244.1	5555.65	5553.81		
Composition (lb/hr)					
HDMA	1.144	5555.65	1.144		
ADA	7101.76	0	7101.76		
H2O	5141.16	0	5141.6		
NYLON66	TRACE	0	TRACE		
Temperature (K):	450	450	450		
Design Data: Operatin	g pressure: 10atm				
Material	: Stainless Steel				
Flow Rat	e:				
Utilities:					
Controls:					
Tolerances:					
NOTE: known simulator i	ssues present				

Mixer3				
Identification: Item	Piping Tee			
No. requi	red 1		Date: 2 March 2017	
			By: David Jacobson	
Function: Facilitate the mixing of waste steam streams				
Operation: Continuous				
Materials handled	VENT2	Recycle1	P3A-C	
Quantity (lb/hr)	6851.55	6860.58 Insignificant		
Composition (lb/hr)				
HDMA	1.53	1.53		
ADA	3.81	3.84		
H2O	6846.21	6855.27		
NYLON66	TRACE	TRACE		
Temperature (K):	600	600	600	
Design Data: Operating	g pressure: 1 atm			
Material:	Carbon Steel			
Flow Rate	2:			
Utilities:				
Controls:				
Tolerances:				

Splitter1					
Identification: Item	Piping 3 way spl	it			
No. require	d 1		Da	te: 2 March 2017	
			By	: David Jacobson	
Function: split flow between	n CSTR reactors				
Operation : Continuous					
Materials handled	P2	P2A	P2B	P2C	
Quantity (lb/hr)		1655.3	1655.3	1655.3	
Composition (lb/hr)					
HDMA	0.0141184	0.00470615	0.00470615	0.00470615	
ADA	0.4524699	0.1508232	0.1508232	0.1508232	
H2O	7.448501	2.482831	2.482831	2.482831	
NYLON66	10940.25	3646.746	3646.746	3646.746	
Temperature (K):	600	600	600	600	
Design Data: Operating p	ressure: 1 atm				
Material: Ca	irbon Steel				
Flow Rate: 119.25 Ft3/HR					
Utilities:					
Controls:					
Tolerances:					

Splitter2					
Identification: Item	Piping Tee				
No. require	d 1	Date: 2 March 201			
			By: David Jacobson		
Function: Separate Recycle	and purge steam stream				
Operation : Continuous					
Materials handled	Cond Rec	Cond H20	WasteH2O		
Quantity (lb/hr)	6860.58	5145.18	1713.80		
Composition (lb/hr)					
HDMA	1.53	1.14	0.38		
ADA	3.83	2.87	0.95		
H2O	6855.22	5141.16	1713.80		
NYLON66	TRACE	TRACE	TRACE		
Temperature (K):	370	370	370		
Design Data: Operating p	ressure: 1 atm				
Material: Ca	arbon Steel				
Flow Rate: 2	208.65 Ft3				
Utilities:					
Controls:					
Tolerances:					

Heat 1					
Identification:	Item	Electric heater			
	No. required	1		Date: 2 March 2017	
				By: David Jacobson	
Function: Supp	ly energy durin	g startup to help brir	ng system to steady state		
Operation: Star	rtup				
Materials hand	led: NA				
Design Data:	Max Power Ra	ating: 500KW			
Utilities:	Electricity				
Controls:					
Tolerances:					

HEAT 2					
Identification: Item	Heat Exchanger				
No. requi	ired 1		Date: 2 March 2017		
By: David			By: David Jacobson		
Function: Provide heat fr	om waste steam streams t	to melt HDMA, and heat	Adipic acid H2O soln.		
Operation: Continuous					
Materials handled	RECYC1-3	COND-REC			
Quantity (lb/hr)	6860.58	6860.58			
Composition (lb/hr)					
HDMA	1.53	1.53			
ADA	3.83	3.83			
H2O	6855.2	6855.2			
NYLON66	TRACE	TRACE			
Temperature (K):	380	370			
Design Data: Operating	g pressure: 1 atm				
Material:	Carbon Steel				
Flow Rate	2:				
Heat Duty: 1409 kW					
Utilities:					
Controls:					
Tolerances:					

	HEAT 3					
Identification: Item	Heat Exchanger					
No. requ	ired 1		Date: 2 March 2017			
			By: David Jacobson			
Function: Heat the ADA	water stream to 450K					
Operation : Continuous						
Materials handled	HOT-ADA	FEEDADA				
Quantity (lb/hr)	12244.1	12244.1				
Composition (lb/hr)						
HDMA	1.144	1.144				
ADA	7101.76	7101.76				
H2O	5141.6	5141.6				
NYLON66	TRACE	TRACE				
Temperature (K):	417	450				
Design Data: Operatir	g pressure: 1 atm					
Material: Carbon Steel						
Flow Rat	e: 207.838 Ft3/hr					
Heat Dut	ty: 172.9 kW					
Utilities: Boiler W	/ater					
Controls:						
Tolerances:						

HX1							
Identification:	fication: Item Heat Exchanger						
No. required 1				Date: 2 Mar	ch 2017		
						By: David J	acobson
Function: Prov	ide heat fr	om waste steam str	eams ⁻	to heat ADA-H	420.		
Operation: Cor	ntinuous						
Materials hand	lled	RECYCLE1	RE	CYCLE1-2	PRES-ADA	HOT	·ADA
Quantity (II	o/hr)	6860.58	68	60.58	12244.06	1224	4.06
Compositio	on (lb/hr)						
HDMA		1.53	1.5	53	1.144	1.144	ŀ
ADA		3.83	3.8	33	7101.76	7101	.76
H2O		6855.2	68	55.2	5141.16	5141	.16
NYLON66		TRACE	TR	ACE	Trace	Trace	5
Temperature (K):	600	47	0	372	417	
Design Data:	Operatin	g pressure: 1 atm					
	Material	: Carbon Steel Shell,	Stainl	ess Steel Tube	es		
	Shell Side	e Flow Rate: 299544	Ft3/h	r			
	Tube Sid	e Flow Rate: 198 Ft3	3/hr				
	Shell Side	e Phase: Vapor					
	Tube Sid	e Flow Rate: Liquid					
	Heat Dut	y: 214.8 kW					
Area: 1.68 m3							
Utilities:							
Controls:							
Tolerances:							

HX2						
Identification:	Item	Heat Exchan	ger			
No. required 1				D	ate: 2 March 2017	
By: David Jacobs						
Function: Provid	de heat fr	om waste steam str	eams to heat HMD	Α.		
Operation: Con	tinuous			1		
Materials handl	led	RECYCLE1-2	RECYCLE1-3	PRES-HDMA	HOT-HDMA	
Quantity (lb	/hr)	6860.58	6860.58	12244.06	12244.06	
Composition	n (lb/hr)					
HDMA		1.53	1.53	5555.65	555.65	
ADA		3.83	3.83	0	0	
H2O		6855.2	6855.2	0	0	
NYLON66		TRACE	TRACE	0	0	
Temperature (K	():	470	380	326.5	450	
Design Data:	Operatin	g pressure: 1 atm				
	Material	: Carbon Steel				
	Shell Side	e Flow Rate: 234200	Ft3/hr			
	Tube Sid	e Flow Rate: 198 Ft3	B/hr			
	Shell Side	e Phase: Liquid				
	Tube Sid	e Flow Rate: Vapor				
Heat Duty: 188.16 kW						
Area: 1.68 m3						
Utilities:						
Controls:						
Tolerances:						

Reactor2A-C				
Identification: Item	CSTR			
No. requ	ired 3		Date: 2 March 2017	
			By: David Jacobson	
Function: To provide add	litional residence time and	d favorable conditions to	o increase nylon MW	
Operation : Continuous				
Materials handled	P2A-C	РЗА-С	VENT3A-C	
Quantity (lb/hr)	3649.39	3649.39	3.00	
Composition (lb/hr)				
HDMA	0.01	0.01	7.26846E-05	
ADA	0.15	0.62	0.00674236	
H2O	2.48	2.49	3.002767	
NYLON66	3646.75	3643.26	3.3613E-78	
Temperature (K):	600	600	600	
Design Data: Operatin	g pressure: 1 atm			
Material	: Carbon Steel			
Flow Rate: 69.55 ft3/hr				
Volume:	10m3			
Utilities:				
Controls:				
Tolerances:				

Reactor1				
Identification: It	tem	PFR		
N	No. required	1		Date: 2 March 2017
				By: David Jacobson
Function: To facil	litate conversi	on of nylon salt to lo	w molecular weight nylon	
Operation: Contin	nuous			
Materials handle	d	MIX1	P1	
Quantity (lb/ł	hr)	17799.71	17799.71	
Composition	(lb/hr)			
HDMA		5556.79	1.54	
ADA		7101.76	4.26	
H2O		5141.16	6853.66	
NYLON66		TRACE	10940.25	
Temperature (K):		450K	555K	
Design Data: C	Operating pres	sure: 10 atm		
Material: Stainless Steel				
F	low Rate: 650	ft3/hr		
L	ength: 50m.			
C	Diameter 1: 0.4	15m		
C	Diameter 2: 0.6	Sm		
F	leat Duty: 339	7.9 kW		
Utilities:	Boiler Water			
Controls:				
Tolerances:				

Flash 1					
Identification: It	tem Flas	sh Drum			
N	lo. required 1			Date: 2 March 2017	
				By: David Jacobson	
Function: To remo	ove water from ny	lon exiting the PFR			
Operation: Contin	nuous				
Materials handled	d P	1	Vent2	P2	
Quantity (lb/h	nr) 1	7799.71	6851.548	10948.17	
Composition ((lb/hr)				
HDMA	1	.54	1.53	0.01	
ADA	4	.26	3.81	0.45	
H2O	H2O 6853.66		6846.21	7.45	
NYLON66	1	0940.25	TRACE 10940.25		
Temperature (K):	5	55K	600k	600	
Design Data: O	Operating pressure	: 5 atm			
N	/laterial: Carbon St	teel			
Flow Rate: 299151 ft3/hr					
Volume: 0.2m3					
Н	leat Duty: 282.68	kW			
Utilities: E	Boiler Water				
Controls:					
Tolerances:					

Dust Collector				
Identification:	ltem	Dust Collector		
	No. required	1		Date: 2 March 2017
				By: David Jacobson
Function: Keep	Function: Keep dust levels low to prevent inhalation hazards, explosion hazards			
Operation: Cor	ntinuous			
Design Data:	Operating pres	ssure: 1 atm		
	Material: Carb	on Steel		
	Volume: 30m3			
Utilities:	electricity			
Controls:				
Tolerances:				

Hopper				
Identification:	ltem	Hopper		
	No. required	2		Date: 2 March 2017
				By: David Jacobson
Function: Feed	s solid HDMA a	nd ADA		
Operation: Cor	ntinuous			
Design Data:	Operating pre	ssure: 1 atm		
	Material: Carb	on Steel		
Utilities:	electricity			
Controls:				
Tolerances:				

Extruder				
Identification:	Item	Extruder		
	No. required	1		Date: 2 March 2017
				By: David Jacobson
Function: solid	ify and granulat	e nylon produc	t	
Operation: Cor	ntinuous			
Design Data:	Operating pres	ssure: 1 atm		
	Material: Carb	on Steel		
Utilities:	electricity			
Controls:				
Tolerances:				

Section 11: Equipment Cost Summary

Equipment	number of equipment	total price (\$)	Base Price
HEAT1	1	10000	10000
HEAT2	2	115886.209	12790.972
HEAT3	1	12918.43002	12918.43
HX1	1	12918.43002	2827.4781
HX2	1	34214.35462	10331.655
BOILER	1	715580.426	715580.43
CSTR	3	911861.6826	100981.36
PFR	1	1099918.428	269984.89
FLASH DRUM	1	82320.84635	27349.118
FEED VESSEL	2	33772.65491	5610.0756
mixers	3	0	0
PUMP 1	1	15315.30089	21479.999
PUMP 2	1	22401.99409	4484.8837
splitter	2	0	0
dust collector	1	42083.12343	42075.567
hopper	2	6000	3000
extruder	1	42000	42000
Total	25	3157191.88	1281414.9

Figure 11.1: Equipment Cost Summary

Section 12: Fixed Capitol Investment Summary

Figure 12.1: Fixed Capitol Investment values

CTM (\$)	3725486.419
base term (\$)	640707.426
CGR (\$)	4366193.844
FCI (\$)	4366193.844

Equation 12.1

$$C_{TM} = 1.18 \sum_{i=1}^{n} C_{BM,i}$$

Equation 12.2

$$C_{GR} = C_{TM} + \frac{1}{2} \sum_{i=1}^{n} C_{BM,i}^{0}$$

 C_{TM} = Total Module Cost C_{BM} = Bare Module Cost C_{GR} = Grass Roots Cost (FCI) C_{BM}^{0} = equipment base price n = number of equipment units in process *Reference: (Source 7)

Description:

The total fixed capital investment (FCI) was determined by calculating the base and bare module costs (See Figure 11.1) for each piece of equipment and using the resulting values in a grass roots plant construction analysis. Equations 12.1 and 12.2, along with the base module and bare module equipment costs provided in Figure 11.1 were used for calculating the FCI by the grass roots method (Turton, 173). It should be noted that this is a general estimate and the author believes it to be an underestimate of the actual capital costs associated with this plant.

Section 13: Safety, Health, and Environmental Considerations

Process Hazard Identification and Address

1) Material Hazards

HMDA and adipic acid are both toxic to humans through ingestion and inhalation. HMDA is also toxic through dermal exposure. Links to MSDS's for both compounds can be found in source 11. Additionally, both compounds are flammable and are capable of forming explosive dust air mixtures when in the solid phase. A dust collector and robust ventilation system will be used to keep dust concentrations below explosive and health exposure limits. Sealed, vented, equipment with antisparking measures will be used to prevent dust concentrations from building up in or around the process as well as to avoid possible ignition sources.

2) Reaction Hazards

HMDA and adipic acid undergo side reactions during the production of nylon to produce basic and acidic vapors as well toxic oligomers. Specific details associated with hazardous reaction by products are given in Appendix A.3. HDMA is also corrosive when mixed with water. Using sealed process vessels will prevent the release of toxic vapors. It is advised that the ventilation system be designed with a scrubber that could be used to neutralize any toxic chemicals in the event of an accidental release. Process equipment exposed to high concentrations of HDMA in water will need to be made out of stainless steel (Source 16).

3) Process Hazards

Multiple pieces of equipment in this process are operated at elevated temperatures and pressures. High pressure vessels pose a mechanical explosion hazard while high temperature vessel can cause severe burns if they leak or are not properly insulated, and can serve as possible ignition sources to flammables. All vessels operated at high pressures will need to be checked regularly to ensure vessel integrity as well as the seals and connections associated with each vessel. A particular emphasis will need to be placed on ensuring that vessels containing high concentrations of HMDA water solutions are not corroding. Vessels operated at high temperatures will also need to be checked for corrosion and vessel integrity, and will need to be insulated or jacketed so that they aren't a potential ignition source for flammables and do not pose burn hazards to individuals in the plant.

Additional Safety Considerations

Although not solely associated with addressing safety issues, a robust process control system will prove key in maintaining process conditions will within the safe operability limit of each piece of equipment. The safe operating conditions of each piece of equipment will need to be well established and then used as upper and lower bounds for controls. Prior to start up, extensive testing will need to be undertaken to determine the sensitivity of conditions in each piece of equipment to different control variable settings, and the general relations between input changes and magnitudes to the effect on the operating conditions of the plant. Such testing protocols will be useful both for ensuring safe operation as well as for optimizing nylon production.

Appropriate levels of personal protection equipment PPE will need to be determined for workers involved in different parts of the plant. Access to respirators will need to be provided in the event of a toxic chemical release of formation of a toxic dust cloud from mishandling of the solid precursors. All personnel will need to be trained both in the use of this PPE as well as how to identify potential process hazards during their job routine.

Environmental Considerations

The largest environmental hazards associated with this process involve a large scale leak of feed materials or process fluid. Calvert City Kentucky is surrounded by large areas of protected wetland that form sensitive ecosystems that could be easily damaged by both small continuous leaks or large chemical spills. Given these consideration, it is advised in this report that process waste water be treated by a third party who specializes in the removal of HDMA, adipic acid, and byproducts of polyamide polymer synthesis, even though waste water solutions are dilute. Particular care will also need to be taken to ensure leaks do not develop within process vessels and chemical storage vessels as well as to ensure that any leaks that do occur can be contained and treated.

In addition to hazards posed by the chemicals involved in this process, particular attention was paid to energy efficiency and reduced water usage during the design of this plant. The choice to use a solid feed melt system rather than a liquid feed enabled a minimization in the amount of waste water generated as well as the amount of energy associated with flashing and heating. The waste steam from the process is used to heat the feed streams and supply the hot water necessary for the dissolution of adipic acid.

Section 14: Other Important Considerations NA

Section 15: Manufacturing Costs

Figure 15.1: Operator Costs

Equipment count*	11
Number of Operators / shift	3
Shift count	4.5
Operator Salary (\$/year)	45000
Operator Costs \$/year	607500

*NOTE: compressors, towers, reactors, heaters, exchangers

Material	price (\$/lb)	yearly material requirements (lbs)	Total Material Cost (\$)
HMDA	1.11	56488121	62701814.31
Adipic Acid	0.67	44917762	30094900.54
Total Cost			92796714.85

Figure 15.3: Waste Treatment Costs

Waste Stream	price (\$/kg)	yearly amount (kg)	yearly cost (\$)
Waste H2O	0.036	6117984	220247.424

Figure 15.4: Direct Manufacturing Costs

Category	Yearly Cost (\$/yr)
Operators	640707
Supervising - clerical	115327.26
maintenance and repairs	260171.58
operating supplies	39025.737
Lab charges	96106.05

Figure 15.5: Fixed Manufacturing Costs

Category	Yearly Cost (\$/yr)
Local taxes and insurance	138758.176
plant overhead costs	586212.948

Figure 15.6: General Expenses

	Yearly Cost
Category	(\$/yr)
Administration	146553.237
distribution and selling costs	12953724.21
research and development	5888056.458

Section 16: Economic Analysis

The full economic analysis of the process is provided in figure 16.2. FCI calculations were carried out using the grass roots method. Manufacturing costs were calculated by the COP method as described by Turton et al. (Source 7). A 130 acre plot of land west of Calvert City Kentucky was selected as an ideal sight for a potential plant (Source 17). The five year MACRS method was used for calculating depreciation.

Based on the calculations presented in figure 16.2, the internal rate of return (IRR) was determined to be 54.5%. Given that a typical hurdle rate for a bulk commodity chemical plant is in the range of 20% to 30%, this plant design appears to be extremely lucrative. It is the recommendation of the author that the fixed capital invest for this plant be further analyzed. 4.3 million dollars is an unusually small value and is likely to be an underestimate. Even if the FCI were to be raised significantly, the earnings potential of this process is quite high compared to other commodity chemical processes.

Further increases in profits could be achieved through process optimization. A more sophisticated method of heat integration that effectively harnesses the energy found within the molten nylon streams (P3A-P3B) would provide significant saving in energy expenditures. It also may be more profitable for the company to make the precursors to nylon on sight (adipic acid and HMDA). The cost of chemical precursors makes up 78% of the manufacturing costs associated with this process. Making the chemicals on sight would require a larger capital investment, but could take advantage of the land already purchased for the nylon plant, share equipment and resources with the nylon plant, and cut out costs associated with the purchase of feed stocks as well as their storage and transport.



Figure 16.1: Cumulative Cash Flow Diagram at IRR

Figure 16.2

	H	urdle	Taxation				n ECI		FCI	1st year		and	Wo	rking	Povonuo	-	` amD	S	alvage		Project	St	art up																																																																																														
	F	Rate	R	ate	r	-CI			L	anu	Ca	pital	Revenue	Ľ			Value		Life		Year																																																																																																
		25.00%	30).00%	\$	4.36	\$	2.91	\$	4.20	\$	1.09	\$130.00	\$	117.00	\$	-		10		2.00																																																																																																
				and	Wo	rking								(RE)			Cash	C	umulative	Dier	ounted	Discou	inted	Po	sitive	Neg	jative																																																																																										
Year	Invo	stment	C	ost	Ca	nital	Den	veciation	FC	l-Dep	Rev	venue	ComD											(REV=COND= DEP)*(1-TAX)								Flow		Flow		Flow				X) Elow		W Cash Flow	Cash Flow Cash Flow			Cumul	ative	Cun	ulative	Cum	ulative																																																																		
	mve	sumern	0	JUSI	Ca	pitai	Dep							DEF	DEP)"(1-TAX)		FIOW C		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW 0		FIOW		FIOW		FIOW		FIOW		FIOW		11000		11000		11000		now		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		FIOW		HOW		1101				1100		FIOW		FIOW				Cash Flow		Cash Plow 10		Cash Flow		Casil Flow		Cash Flow			Cash	Flow	w Discount		Disc	ounted
0	\$	-	\$	(4.20)	\$	-	\$	-	\$	4.36	\$	-	\$-	\$	-	\$	(4.20)	\$	(4.20)	\$	(4.20)	\$	(4.20)	\$	-	\$	(4.20)																																																																																										
1	\$	(2.91)	\$	-	\$	-	\$	-	\$	4.36	\$	-	\$-	\$	-	\$	(2.91)	\$	(7.11)	\$	(2.33)	\$	(6.53)	\$	-	\$	(6.53)																																																																																										
2	\$	(2.54)	\$	-	\$	(1.09)	\$	-	\$	4.36	\$	-	\$-	\$	-	\$	(2.54)	\$	(9.65)	\$	(1.63)	\$	(8.15)	\$	-	\$	(8.15)																																																																																										
3	\$	-	\$	-	\$	-	\$	0.87	\$	3.49	\$1	30.00	\$117.00	\$	9.36	\$	9.36	\$	(0.29)	\$	4.79	\$	(3.36)	\$	4.79	\$	(8.15)																																																																																										
4	\$	-	\$	-	\$	-	\$	1.40	\$	2.09	\$1	30.00	\$117.00	\$	9.52	\$	9.52	\$	9.23	\$	3.90	\$	0.54	\$	8.69	\$	(8.15)																																																																																										
5	\$	-	\$	-	\$	-	\$	0.84	\$	1.26	\$1	30.00	\$117.00	\$	9.35	\$	9.35	\$	18.58	\$	3.06	\$	3.60	\$	11.76	\$	(8.15)																																																																																										
6	\$	-	\$	-	\$	-	\$	0.50	\$	0.75	\$1	30.00	\$117.00	\$	9.25	\$	9.25	\$	27.83	\$	2.43	\$	6.03	\$	14.18	\$	(8.15)																																																																																										
7	\$	-	\$	-	\$	-	\$	0.50	\$	0.25	\$1	30.00	\$117.00	\$	9.25	\$	9.25	\$	37.08	\$	1.94	\$	7.97	\$	16.12	\$	(8.15)																																																																																										
8	\$	-	\$	-	\$	-	\$	0.25	\$	0.00	\$1	30.00	\$117.00	\$	9.18	\$	9.18	\$	46.26	\$	1.54	\$	9.51	\$	17.66	\$	(8.15)																																																																																										
9	\$	-	\$	-	\$	-	\$	-	\$	-	\$1	30.00	\$117.00	\$	9.10	\$	9.10	\$	55.36	\$	1.22	\$	10.73	\$	18.88	\$	(8.15)																																																																																										
10	\$	-	\$	-	\$	-	\$	-	\$	-	\$1	30.00	\$117.00	\$	9.10	\$	9.10	\$	64.46	\$	0.98	\$	11.71	\$	19.86	\$	(8.15)																																																																																										
11	\$	-	\$	-	\$	-	\$	-	\$	-	\$1	30.00	\$117.00	\$	9.10	\$	9.10	\$	73.56	\$	0.78	\$	12.49	\$	20.64	\$	(8.15)																																																																																										
12	\$	5.29	\$	-	\$	1.09	\$	-	\$	-	\$1	35.29	\$117.00	\$	12.80	\$	18.09	\$	91.65	\$	1.24	\$	13.73	\$	21.88	\$	(8.15)																																																																																										

Section 17: Conclusions and Recommendations

It is the opinion of the author that the nylon 6 6 production process presented in this report possesses significant earnings potential that should warrant additional investigation into its feasibility as well as consideration for investment. This report constitutes an initial low cost design and economic feasibility study. Review of this report by additional design engineers is highly encouraged as well as additional research into process optimization, safety considerations, and process control schemes. Although additional research will be costly the high IRR value (54.5%) associated with the initial estimate of the cost of this process should justify the decision to pursue this project further. Section 18: Acknowledgements

This work was undertaken as a part of the Chemical Engineering Design 2 class at the University of Arkansas during the spring of 2017. Simulator access was provided by the University of Arkansas Chemical Engineering Department. Data base access was provided by the University of Arkansas library system.

Section 19: Bibliography

Source 1

Giudici R, Nascimiento C (1999) Mathematical modeling of an industrial process of nylon-6,6 polymerization in a two-phase flow tubular reactor. Chem Eng Sci 54(15–15):3243–3249

Source 2

Giudici R (2006) Simulation model of polyamide-6,6 polymerization in a continuous two-phase flow coiled tubular reactor. Ind Eng Chem Res 45:4558–4566

Source 3 Kumar A, Gupta R (2003) Fundamentals of polymers, 2nd edn. McGraw Hill, New York, Chapter 4

Source 4 Seavey K, Liu YA (2008) Step-growth polymerization process modeling and product design. Wiley, New York, Chapter 15

Source 5 Wakabayashi C (2008) Fuzzy control of a nylon polymerization semi-batch reactor. Fuzzy Sets Syst 160(4):537–553

Source 6 Van Krevelen D (2009) Properties of polymers, 4th edn. Elsevier, Amsterdam

Source 7

Turton, R. (2009). *Analysis, synthesis, and design of chemical processes*. Upper Saddle River, N.J: Prentice Hall.

Source 8 http://www.chemengonline.com/current-economic-trends-march-2016/?printmode=1 CEPCI

Source 9 http://www.electricitylocal.com/states/kentucky/

Source 10 https://www.eia.gov/dnav/ng/hist/n3035ky3m.htm

Source 11 MSDS's Adipic Acid: <u>http://www.sciencelab.com/msds.php?msdsId=9927423</u> HMDA: <u>http://www.sciencelab.com/msds.php?msdsId=9924250</u>

Source 12 https://www.alibaba.com/product-detail/polymer-resin-pellets-extrusionmachine 60596706053.html?s=p Source 13

https://www.alibaba.com/product-detail/Stainless-Steel-Tubular-Screw-Conveyor-With 60527625845.html?spm=a2700.7724838.0.0.y9yiAU

Source 14

http://www.mypurchasingcenter.com/commodities/commodities-articles/nylon-price-forecast-2015/

Source 15 HDMA / ADIPIC ACID PRICE: Invista

Source 16 http://hayata.com/stainless-steel-chemical-resistance-chart-ab/

Source 17 http://www.landwatch.com/Marshall-County-Kentucky-Land-for-sale/pid/3637403

*Authors Note: Internet sources are referenced here in an informal manner due to the variety of web pages being referenced that do not conform to formats associated with typical academic sourcing. Any additional information needed from these sources can be obtained by contacting the author

Section 20: Appendix

A.1: Solubility Calcs and references

required mass of hdma	solubility of HDMA (Kg/L) (roomtemp	required water (Kg/hr)						
(kg)	water)							
2520	2.46	1024						
	https://pubchem.ncbi.nlm.nih.gov/compound/1_6-							
	Hexanediamine#section=Flash-Point							
required mass of ADA	solubility (Kg/L) (boiling water)	required water (kg/hr)						
(kg)								
3220	1.6	2236.111111						
	https://pubchem.ncbi.nlm.nih.gov/compound/adipic_acid#section=Solu							
	у							

A.2: Process Tables

Stroom			COND-	CONDUZO						NALV1
Stream	ADA	ADAHZO	REC	CONDH20	FEEDADA	FEEDHDIVIA	HUT-ADA	HUTHDIMA	LIQHDIMA	
Downstream Block	MIXER1	PUMP2	SPLIT2	MIXER1	MIXER2	MIXER2	HEAT3	HEAT1	PUMP1	R1
Upstream block		MIXER1	HEAT2	SPLIT2	HEAT3	HEAT1	HX1	HX2		MIXER2
Phase	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MIXED
Mass Flow kg/hr										
HMDA	0	0.5189741	0.6918947	0.5189741	0.5189741	2520	0.5189741	2520	2520	2520.519
ADA	3220	3221.304	1.738618	1.303815	3221.304	0	3221.304	0	0	3221.304
H2O	0	2331.991	3109.474	2331.991	2331.991	0	2331.991	0	0	2331.991
NYLON66	0	3.24E-75	4.32E-75	3.24E-75	3.24E-75	0	3.24E-75	0	0	3.24E-75
Total Flow kg/hr	3220	5553.814	3111.905	2333.814	5553.814	2520	5553.814	2520	2520	8073.814
Vapor Frac	0	0	0	0	0	0	0	0	0	0.230327
Liquid Frac	1	1	1	1	1	1	1	1	1	0.769673
Solid Frac	0	0	0	0	0	0	0	0	0	0
Temperature K	373	371.324	370	370	450	450	416.4789	449.9999	325	384.4021
Pressure atm	1	1	10	10	10	10	10	10	1	1
Enthalpy J/kg	-6.48E+06	-1.03E+07	-1.55E+07	-1.55E+07	-1.00E+07	-9.71E+05	-1.01E+07	-9.71E+05	-1.24E+06	-7.20E+06
Entropy J/kg-K	-4859.427	-6143.825	-8139.866	-8139.866	-5536.388	-6955.823	-5785.265	-6955.823	-7657.854	-5849.884
Average MW	146.143	36.66083	18.0275	18.0275	36.66083	116.2065	36.66083	116.2065	116.2065	46.62166
NYLON66 SFRAC										
HMDA-E		5.72E-03	5.72E-03	5.72E-03	5.72E-03		5.72E-03			5.72E-03
ADA-E		0.0215022	0.0215027	0.0215022	0.0215022		0.0215022			0.0215022
HMDA-R		0.4903317	0.4903326	0.4903317	0.4903317		0.4903317			0.4903317
ADA-R		0.4824424	0.4824423	0.4824424	0.4824424		0.4824424			0.4824424
NYLON66 DPN										
DPN		73.45944	73.46165	73.45944	73.45944		73.45944			73.45944
NYLON66 MWN										
MWN		8339.322	8339.574	8339.322	8339.322		8339.322			8339.322

A.2: Process Tables (cont.)

P1	P2	P2A	P2B	P2C	P3A	P3B	P3C	PRES-ADA	PRESHDMA	RECYC1-2	RECYC1-3
FLASH1	SPLIT1	R2A	R2B	R2C				HX1	HX2	HX2	HEAT2
R1	FLASH1	SPLIT1	SPLIT1	SPLIT1	R2A	R2B	R2C	PUMP2	PUMP1	HX1	HX2
MIXED	LIQUID	VAPOR	MIXED								
0.6981982	6.40E-03	2.13E-03	2.13E-03	2.13E-03	2.34E-04	2.34E-04	2.34E-04	0.5189741	2520	0.6918947	0.6918947
1.934684	0.2052369	0.0684122	0.068413	0.0684116	0.2809715	0.2809748	0.280969	3221.304	0	1.738618	1.738618
3108.767	3.378583	1.126193	1.126207	1.126183	1.130891	1.130904	1.13088	2331.991	0	3109.474	3109.474
4962.414	4962.414	1654.136	1654.156	1654.122	1652.556	1652.576	1652.541	3.24E-75	0	4.32E-75	4.32E-75
8073.814	4966.005	1655.333	1655.353	1655.318	1653.968	1653.988	1653.953	5553.814	2520	3111.905	3111.905
0.8733585	0	0	0	0	0	0	0	0	0	1	0.9860001
0.1266415	1	1	1	1	1	1	1	1	1	0	0.0139999
0	0	0	0	0	0	0	0	0	0	0	0
555	600	600	600	600	599	599	599	372.0078	326.5722	470	373.3258
8	1	1	1	1	1	1	1	10	10	1	1
-5.69E+06	-1.01E+06	-1.01E+06	-1.01E+06	-1.01E+06	-1.00E+06	-1.00E+06	-1.00E+06	-1.03E+07	-1.24E+06	-1.31E+07	-1.33E+07
-3687.38	-4341.45	-4341.45	-4341.45	-4341.45	-4347.586	-4347.586	-4347.586	-6136.493	-7646.572	-1608.855	-2136.45
41.50876	224.5472	224.5472	224.5472	224.5472	224.523	224.523	224.523	36.66083	116.2065	18.0275	18.0275
5.73E-03	5.73E-03	5.73E-03	5.73E-03	5.73E-03	5.24E-04	5.24E-04	5.24E-04	5.72E-03		5.72E-03	5.72E-03
0.0215085	0.0215085	0.0215085	0.0215085	0.0215085	0.016101	0.016101	0.016101	0.0215022		0.0215027	0.0215027
0.490327	0.490327	0.490327	0.490327	0.490327	0.4955821	0.4955821	0.4955821	0.4903317		0.4903326	0.4903326
0.4824367	0.4824367	0.4824367	0.4824367	0.4824367	0.4877934	0.4877934	0.4877934	0.4824424		0.4824423	0.4824423
73.43124	73.43124	73.43124	73.43124	73.43124	120.3041	120.3041	120.3041	73.45944		73.46165	73.46165
8336.129	8336.129	8336.129	8336.129	8336.129	13645.59	13645.59	13645.59	8339.322		8339.574	8339.574

A.2: Process Tables (cont.)

		,			
RECYCLE1	VENT2	VENT3A	VENT3B	VENT3C	WASTEH20
HX1	MIXER3	MIXER3	MIXER3	MIXER3	
MIXER3	FLASH1	R2A	R2B	R2C	SPLIT2
VAPOR	VAPOR	VAPOR	VAPOR	VAPOR	LIQUID
0.6918947	0.6917942	3.30E-05	3.30E-05	3.30E-05	0.1729737
1.738618	1.729447	3.06E-03	3.06E-03	3.06E-03	0.4346546
3109.474	3105.388	1.362032	1.362049	1.36202	777.3686
4.32E-75	4.31E-75	1.52E-78	1.52E-78	1.52E-78	1.08E-75
3111.905	3107.81	1.365124	1.36514	1.365111	777.9763
1	1	1	1	1	0
0	0	0	0	0	1
0	0	0	0	0	0
599.9987	600	599	599	599	370
1	1	1	1	1	10
-1.28E+07	-1.28E+07	-1.28E+07	-1.28E+07	-1.28E+07	-1.55E+07
-1125.145	-1125.139	-1129.977	-1129.977	-1129.977	-8139.866
18.0275	18.02747	18.0511	18.0511	18.0511	18.0275
5.72E-03	5.73E-03	5.24E-04	5.24E-04	5.24E-04	5.72E-03
0.0215027	0.0215085	0.016101	0.016101	0.016101	0.0215027
0.4903326	0.490327	0.4955821	0.4955821	0.4955821	0.4903326
0.4824423	0.4824367	0.4877934	0.4877934	0.4877934	0.4824423
73.46165	73.43124	120.3041	120.3041	120.3041	73.46165
8339.574	8336.129	13645.59	13645.59	13645.59	8339.574

A.3: Cameo Chemicals Chemical Compatibility Report



Chemical Reactivity

Substances In The Mix

- 1. HEXAMETHYLENEDIAMINE, SOLID
- 2. ADIPIC ACID
- 3. HEXAMETHYLENEDIAMINE, SOLUTION
- 4. WATER

▲ Summary of Hazard Predictions (for all pairs of sunstances)

- Corrosive: Reaction products may be corrosive
- Generates gas: Reaction liberates gaseous products and may cause pressurization
- Generates heat: Exothermic reaction at ambient temperatures (releases heat)
- Toxic: Reaction products may be toxic

ASummary of Gas Predictions (for all pairs of sunstances)

May produce the following gases:

- Acid Fumes
- Base Fumes

Hazard Predictions (for each pair of substances)

ADIPIC ACID *mixed with* HEXAMETHYLENEDIAMINE, SOLID

- Corrosive: Reaction products may be corrosive
- Generates gas: Reaction liberates gaseous products and may cause pressurization
- Generates heat: Exothermic reaction at ambient temperatures (releases heat)
- **Toxic:** Reaction products may be toxic
- May produce the following gases:
 - Acid Fumes
 - Base Fumes

HEXAMETHYLENEDIAMINE, SOLUTION *mixed with* HEXAMETHYLENEDIAMINE, SOLID

• Corrosive: Reaction products may be corrosive

HEXAMETHYLENEDIAMINE, SOLUTION mixed with ADIPIC ACID

- Corrosive: Reaction products may be corrosive
- Generates gas: Reaction liberates gaseous products and may cause pressurization
- Generates heat: Exothermic reaction at ambient temperatures (releases heat)
- **Toxic:** Reaction products may be toxic
- May produce the following gases:
 - Acid Fumes
 - Base Fumes

WATER *mixed with* HEXAMETHYLENEDIAMINE, SOLID

• Corrosive: Reaction products may be corrosive

WATER *mixed with* ADIPIC ACID

• No known hazardous reaction

WATER *mixed with* HEXAMETHYLENEDIAMINE, SOLUTION

• **Corrosive:** Reaction products may be corrosive