4-2013

A Green Process for Niacinamide Production

Praveen Bains
University of Pennsylvania

Ashley Clark
University of Pennsylvania

Amber Lowey
University of Pennsylvania

Jamie Soo
University of Pennsylvania

A Green Process for Niacinamide Production

Abstract
This project proposes a plant in which niacinamide can be produced with an environmentally green process. Specifically, it takes 2-methyl-1,5-pentanediamine (MPDA) as a starting reactant and converts it to picoline before subsequently converting it to niacinamide and purifying the final product. By following this particular reaction path, the process avoids the more classic method of preparation by which nicotine is oxidized with potassium dichromate, a reaction with considerably more toxic reactants and waste. Along with this more sustainable reaction path, care was taken to ensure the process was as green as possible at each step along the way.

The primary global supplier of niacin is Lonza, whose patent provided the base upon which this process was developed. Only preliminary data was furnished by the patent; the majority of the process presented within this portfolio was developed with limited information from the patent reference.

The base-case process presented in this project consists of three main sections; Block 100 involves the conversion of MPDA into picoline, Block 200 involves the formation of niacinamide from picoline, and Block 300 involves the separation and purification of the niacinamide into the final marketable product. A final purity of 97.7% by weight was achieved. Rigorous economic analysis was performed on the entirety of the process, yielding an NPV of $4,932,800 after 20 years and an internal rate of return (IRR) of 16.82% after the third year. Although each of these indicate a positive return on investment, as the economic success of this process is highly subject to the market value of both the feedstock MPDA and product niacinamide, further investigation may be necessary before final project approval.

Disciplines
Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

A GREEN PROCESS FOR NIACINAMIDE PRODUCTION

Praveen Bains
Ashley Clark
Amber Lowey
Jamie Soo

University of Pennsylvania
School of Engineering and Applied Sciences
Chemical and Biomolecular Engineering

April 9, 2013

University of Pennsylvania
School of Engineering and Applied Science
Department of Chemical and Biomolecular Engineering
220 South 33rd Street
Philadelphia, PA 19104

April 9, 2013

Dear Mr. Fabiano and Dr. Holleran,

Enclosed is our proposed process design for the green production of niacinamide from an environmentally friendly facility, as specified in a problem statement by Mr. Fabiano. Our plant design entails two reaction sections and a separation train to obtain 97.7% by weight final product purity. We have also designed a Dowtherm distribution system to help achieve our heating requirements throughout the system.

Our finalized process includes three distinct sections. In the first, 2-methyl-1,5-pentanediamine is converted to 3-picoline, in the second section 3-picoline is converted to the desired product niacinamide, and the third separates and purifies the final product. By utilizing the raw material of 2-methyl-1,5-pentanediamine, this process is able to avoid the formation of harsh intermediates like acrolein and is significantly more sustainable and environmentally conscientious than previous niacin production processes.

The following report details the specifics of the process, the equipment needs for each stage of the process, the estimated costs and power requirements of each piece of equipment, and a detailed economic analysis of the overall process.

Detailed economic analyses, including sensitivities to key costing parameters, have been included. Environmental concerns and waste streams have been evaluated. Overall, the process is profitable with a return on investment of approximately 11.09%. However, this analysis is very sensitive to the market prices of both 2-methyl-1,5-pentanediamine and niacinamide in addition to requiring 14 years before a return on the investment can be collected.

Sincerely,

Praveen Bains

Ashley Clark

Amber Lowey

Jamie Soo

Table of Contents

I. Abstract

A. ABSTRACT

This project proposes a plant in which niacinamide can be produced with an environmentally green process. Specifically, it takes 2-methyl-1,5-pentanediamine (MPDA) as a starting reactant and converts it to picoline before subsequently converting it to niacinamide and purifying the final product. By following this particular reaction path, the process avoids the more classic method of preparation by which nicotine is oxidized with potassium dichromate, a reaction with considerably more toxic reactants and waste. Along with this more sustainable reaction path, care was taken to ensure the process was as green as possible at each step along the way.

The primary global supplier of niacin is Lonza, whose patent provided the base upon which this process was developed. Only preliminary data was furnished by the patent; the majority of the process presented within this portfolio was developed with limited information from the patent reference.

The base-case process presented in this project consists of three main sections; Block 100 involves the conversion of MPDA into picoline, Block 200 involves the formation of niacinamide from picoline, and Block 300 involves the separation and purification of the niacinamide into the final marketable product. A final purity of 97.7% by weight was achieved. Rigorous economic analysis was performed on the entirety of the process, yielding an NPV of $4,932,800 after 20 years and an internal rate of return (IRR) of 16.82% after the third year. Although each of these indicate a positive return on investment, as the economic success of this process is highly subject to the market value of both the feedstock MPDA and product niacinamide, further investigation may be necessary before final project approval.

II. Introduction and Project Charter

A. PROJECT CHARTER

Project Name A Green Process for Niacinamide Production

Project Champion Professor Leonard A. Fabiano, U. Penn

Project Advisor Dr. Sean P. Holleran, U. Penn

Project Leaders Praveen Bains, Ashley Clark, Amber Lowey, Jamie Soo

Specific Goals Design and determine the economic viability of a plant that produces competitive amounts of niacinamide to capture an equivalent amount of market share of niacinamide as the Lonza company

Project Scope

In Scope

- Determining the world market for niacin and the current worldwide production capacity
- Determining the selling price of niacin
- Developing a process design of a facility that produces 27.7 MM lbs/yr niacinamide based on the Lonza process
- Building upon and fully realize the existing process flowsheet described in Lonza's patent
- Completing approximate equipment sizing and costing
- Determining economic viability of the proposed facility
- Producing niacinamide of at least 95 weight % purity

Out of Scope

- Verifying reaction kinetics, conversions, and yields proposed in the Lonza patent
- Developing wastewater treatment facilities, air scrubbing units, Dowtherm heating systems, and refrigeration systems
- Determining safety layout of facilities

Deliverables

- Full Plant Design
- Detailed Economic Analysis
- Approximate Equipment Sizing

Timeline

- Initial process design completed by February 19th, 2013
- Initial equipment sizing completed by March 12th , 2013
- Initial economic analysis completed by March 26th, 2013
- Deliverables completed by April 9th, 2013

B. PROJECT MOTIVATION

This project has been commissioned to produce niacin on a scale capable of being competitive in the world markets and of comparable market share as primary producers such as Lonza or Jubilant. Additionally, this project is intended to explore various methods of reducing the environmental footprint of the overall process and improving its general sustainability. Niacin is important as a supplement for human consumption and as an additive to animal feed. Naturally, these markets have differing standards of purity. The importance of niacin is further discussed in the Market and Competitive Analysis in section IV Concept Stage.

The process that was developed was modeled on the Lonza process patent, a niacin production method which utilizes picoline as an intermediate reactant known for its "green chemistry". This additional step allows the use of acrolein to be avoided, thereby reducing the amount of hazardous intermediates involved. Aside from the reaction process itself, the Lonza process has also established a set of guidelines which encompass nearly every factor of production from choice of feedstock to treatment of wastes, aimed at minimizing the overall footprint of production.

Beyond the adoption of the use of picoline, the Lonza process takes many other green factors into account including the choice of feedstock, the reaction path, and the choice of catalyst. In keeping with these guidelines, manufacture of the process' feedstock should be environmentally friendly, a reaction path should be selected as to minimize the overall energy required by the reaction. The selection of catalyst takes into account means obtained, availability, cost, efficiency (frequency of replacement), and recyclability. In addition to the parameters outlined by the Lonza patent, this project made a specific effort to design a more efficient separation train, to minimize the amount of pollutants and waste streams, and to ensure the proper treatment and disposal of all auxiliary, side, and intermediate products.

Finally, to enter a pre-existing market, the economic feasibility of production must be analyzed. Taking into account overall market capacity, established market prices of both product and feedstock, operating costs and initial capital investment for a determined ideal production rate, the final profitability and return on investment must be calculated.

The project aims to develop a process which improves the environmental impact of production and can thus be simultaneously profitable and environmentally sustainable.

C. METHODS OF PRODUCTION

Patent US5719045 from Lonza served as the basis for our process, providing the reaction pathway and reactor conditions necessary for niacinamide production. A separation and purification process was then designed to obtain the necessary purity for our targeted market of 95% for animal feed. The production begins with a series of four reactor systems: two tubular reactors, one packed-bed reaction, and continuously-stirred tank reactors (CSTRs) in series. The biocatalyst *Rhodococcus rhodocrous* is used in the CSTRs. Hydrogen is separated after the second reactor for use as the Dowtherm system fuel. The slurry product stream then undergoes a single distillation, two flash vaporizers, and concludes at a nitrogen-fed dryer. The result is a final product stream of niacinamide with 97.7 weight % purity as a powder. This is suitable for the animal feed market.

Raw Materials

The raw materials for the process include MPDA, water, oxygen, and nitrogen. The table below denotes the cost of each of these. The cost of MPDA was estimated by dividing the cost of MPDA from Sigma Aldrich by a factor of 10. This factor was determined by comparing bulk and non-bulk prices of other chemicals, such as niacinamide.

Raw Material	**Price ($ /lb)**
MPDA	$3.091
Process Water	$7.5 × 10^{-4}$
Oxygen	$0.035
Nitrogen	$0.050

Table C1. Raw material prices for niacinamide production.

The catalysts were priced according to their composition and were chosen following the suggestions offered by Lonza's patent US5719045. Table C2 lists each catalysts and its price. Please refer to the Sample Catalyst Calculations in Appendix IX for catalyst costing methods.

Catalyst	Total Price ($/)
HZSM-5 (Zeolite)	$3,810
Pd-SiO_2/Al_2O_3	$783,300
V_2O_5/TiO_2/ZrO_2/MoO_3	$1,646,000
Rhodococcus rhodocrous	$153,900

Table C2. Prices of catalysts used in niacinamide production.

Reaction

The reaction pathway proposed by Lonza in the patent US5719045 was followed to produce niacinamide. The Lonza method of niacin production follows two stages with two reactions in each. The first set produces the starting material for niacin production, 3-picoline. The second set oxidizes the picoline to form niacinamide and niacin.

The process begins with MPDA as the starting raw material, which is a byproduct of the nylon-6,6 industry. The liquid MPDA is first vaporized and is converted to 3-methylpiperidine (MPI) via deamination, resulting in a ring closure. This exothermic reaction takes place in the presence of the zeolite catalyst, HZSM-5:

$$[MPDA] \rightarrow [MPI] + [NH_3] \tag{1}$$

The methyl piperidine is then dehydrogenated endothermically to 3-picoline (PIC) over a Pd-SiO_2/Al_2O_3 catalyst:

$$[MPI] \rightarrow [PIC] + 3\,[H_2] \tag{2}$$

During this step, a side reaction converts about 10% of the picoline into various byproducts:

$$2\,[PIC] + 15\tfrac{1}{2}\,[O_2] \rightarrow [N_2] + 12\,[CO_2] + 7\,[H_2O] \tag{3}$$

The remaining picoline undergoes an exothermic ammoxidation V_2O_5/TiO_2/ZrO_2/MoO_3 catalyst to form 3-cyanopyridine (CNP):

$$[PIC] + \frac{3}{2}\,[O_2] + [NH_3] \rightarrow [CNP] + 3\,[H_2O] \tag{4}$$

Finally, a biocatalyst (nitrile hydratase produced by *Rhodococcus rhodocrous J1*) helps to convert the CNP into niacinamide via an enzymatic hydrolysis process.

$$[CNP] + [H_2O] \rightarrow [niacinamide] \tag{5}$$

The yields of niacinamide are determined by adjusting the pH of the fourth reactor, which consists of three CSTRs in series. The products then travel through a separation train to form a high purity, powdered form.

An overview of the reaction steps are shown below, reproduced from a paper written by Roderick Chuck from Lonza.

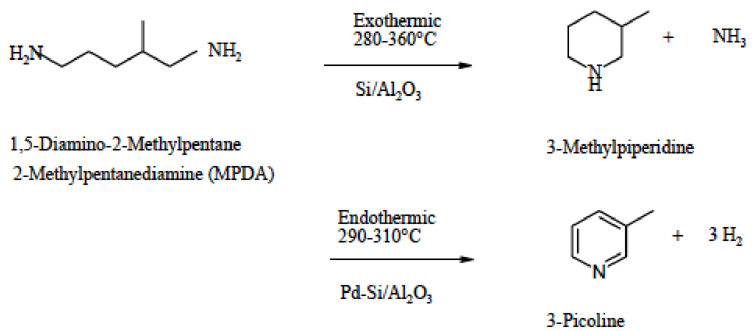


Figure 1. Conversion of MPDA to MPI and MPI to PIC.

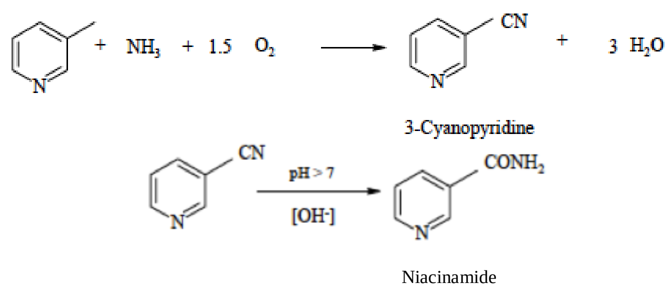


Figure 2. Conversion of PIC to CNP and then CNP to niacinamide.

Sustainability

As mentioned in the introduction, a main motivation for this project is incorporating green or sustainable methods with the process design. Roderick Chuck from Lonza in his paper entitled Technology Development in Nicotinate Production outlined key factors for the patented reaction pathway. The following green advantages were noted: use of air as an oxidant in lieu of another chemical, use of catalysts to increase reaction rate, reaction conditions that allow for the catalyst to be easily regenerated, atmospheric pressure for each reaction, and recoverable energy from the exothermic reactions. While building the niacinamide production process, careful attention was given to increasing its sustainability. In the Lonza patent, the hydrogen gas was burned directly to evaporate the MPDA. In this project, the hydrogen byproduct is separated and sent to fuel a Dowtherm heating system. Dowtherm A is used as a heat transfer fluid that maintains the high temperatures required for the dehydrogenation reaction and other heat exchangers. Wet scrubbers are used to remove the minimal CO2 released during the process. Furthermore, the startup fuel chosen for the Dowtherm system is renewable natural gas, an upgraded version of biogas, which releases less CO2 than natural gas. Renewable natural gas does not require hydraulic fracturing as it is created from biomass. These aspects contribute to the overall sustainability of the niacinamide production process. Additionally, water is the only solvent required, and toxic chemical such as ammonia and Dowtherm A are recycled within the system.

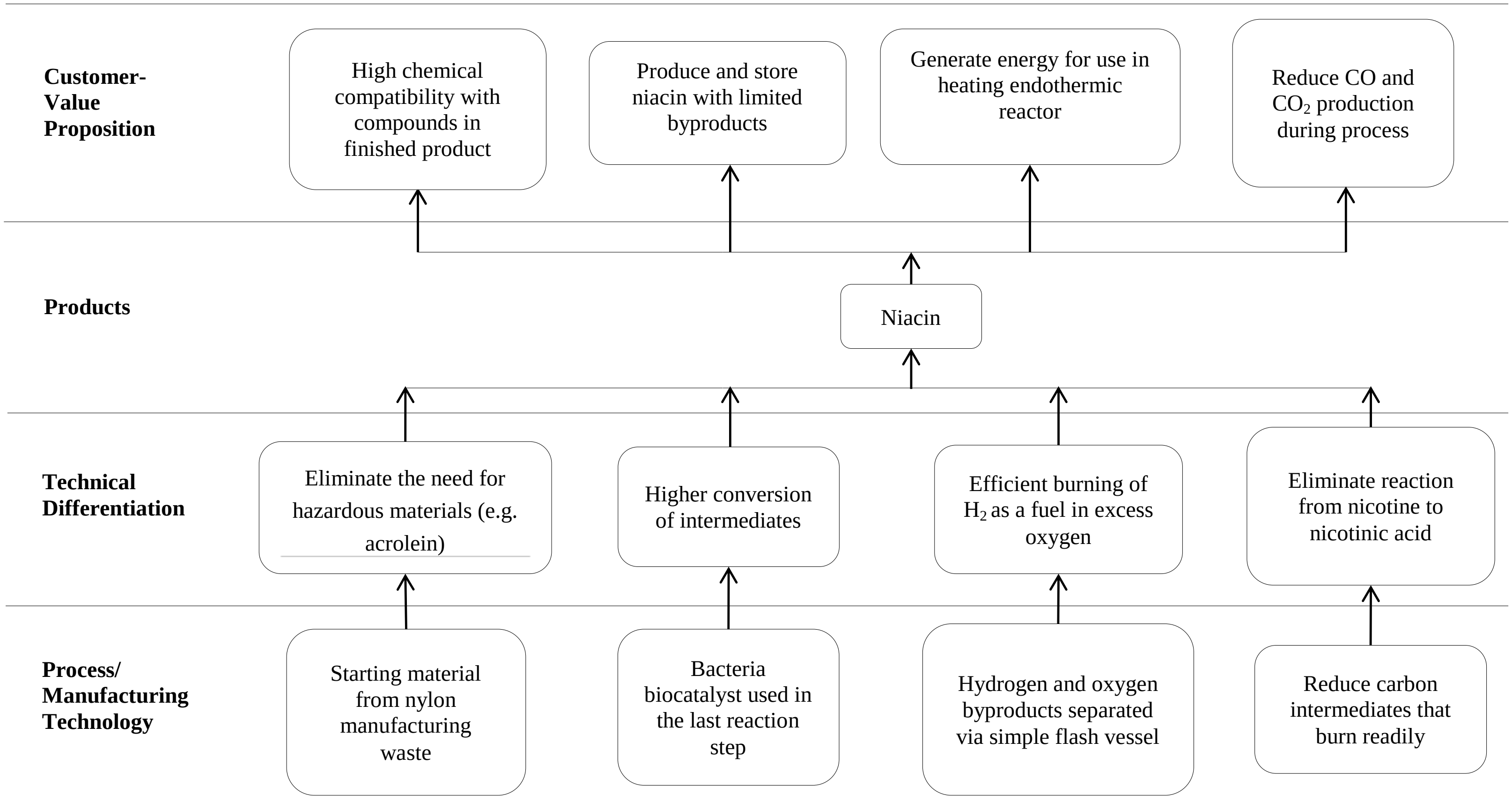
Plant Location

The niacinamide production plant will be located in Michigan, due to its proximity to a producer of the raw material MPDA, Invista. Invista owns a manufacturing plant in Mississauga, Ontario, just across the lake. This will reduce cost of transportation greatly. The proximity of other chemical plants in the area also indicates the availability of utilities for running a process plant. For distribution of the product, this location also offers integration into an existing network of the targeted market, animal feedstock.

Plant Capacity

The plant will produce 3,452 lb/hr of niacinamide at 97.7% purity. The plant will be online for 335 days of the year for a total of 8,026 hours. This results in a yearly output of 27.7 million lbs. Additionally the plant will produce and separate 1.4 million lbs of hydrogen per year for use in the Dowtherm system. The remaining 30 days will be used for maintenance, safety inspections, and catalyst regeneration.

III. INNOVATION MAP


Customer-Value Proposition
High chemical compatibility with compounds in finished product
Produce and store niacin with limited byproducts
Generate energy for use in heating endothermic reactor
Reduce CO and CO_2 production during process
Products
Niacin
Technical Differentiation
Eliminate the need for hazardous materials (e.g. acrolein)
Higher conversion of intermediates
Efficient burning of H_2 as a fuel in excess oxygen
Eliminate reaction from nicotine to nicotinic acid
Process/ Manufacturing Technology
Starting material from nylon manufacturing waste
Bacteria biocatalyst used in the last reaction step
Hydrogen and oxygen byproducts separated via simple flash vessel
Reduce carbon intermediates that burn readily

IV. Concept Stage

A. MARKET AND COMPETITIVE ANALYSIS

The term niacin is commonly used to describe both nicotinic acid and niacinamide. Both of these compounds are water-soluble and are part of the vitamin B group. Nicotinic acid and niacinamide are necessary for all living cells as they are essential contributors to proper carbohydrate, protein and lipid metabolism.

Niacinamide and nicotinic acid are components of the coenzymes niacinamide dinucleotide (NAD) and niacinamide adenine dinucleotide phosphate (NADP), which are both key intermediates in the metabolic process. More than 40 biochemical reactions have been identified that utilize these coenzymes, particularly in relation to the skin, gastrointestinal tract and nervous system. In humans, a deficiency of niacin can result in a wide variety of symptoms, from severe digestive system disorders, to weakness, skin discoloration, loss of appetite, and retarded growth.

Due to its great importance in biological functions, niacin is most commonly used in feed, food, and pharmaceutical industries. The global market size of niacin and niacinamide is over $400 million USD, with an estimated production rate of 20,200 metric ton per year (TPA) or 44,603,000 lbs/yr (Lonza Group, Ltd., 2011). Its largest market demand is as a feed supplement feed for stock animals, accounting for 60-70% of the total market. The remaining 30-40% of the market is divided amongst human nutrition, cosmetics, pharmaceuticals, and other technical applications including the preparation of metal surfaces (Feedinfo News Services, 2012).

The purity necessitated by each of these applications varies greatly, with human consumption demanding the highest purity standards of 99.5%. The top markets, located in North America, Europe, and China, have seen significant growth over the past several years. The overall projected global demand niacin growth over the next few years is 5-7% (Feedinfo News Services, 2012).

The two primary competitors in niacin and niacinamide production are Lonza and Jubilant. Lonza, whose patent was used as a starting point for this project, controls a little more than half of the world's production with a production rate of 10,700 TPA (2,362,000 lbs/yr). Lonza controls three large-scale plants, one operating in Switzerland where the firm is based and two others operating in China (Pharmaceutical-Technology, 2011). Jubilant is based in India, and as of 2011, has a commercial production rate of 10,000 TPA niacinamide per year.

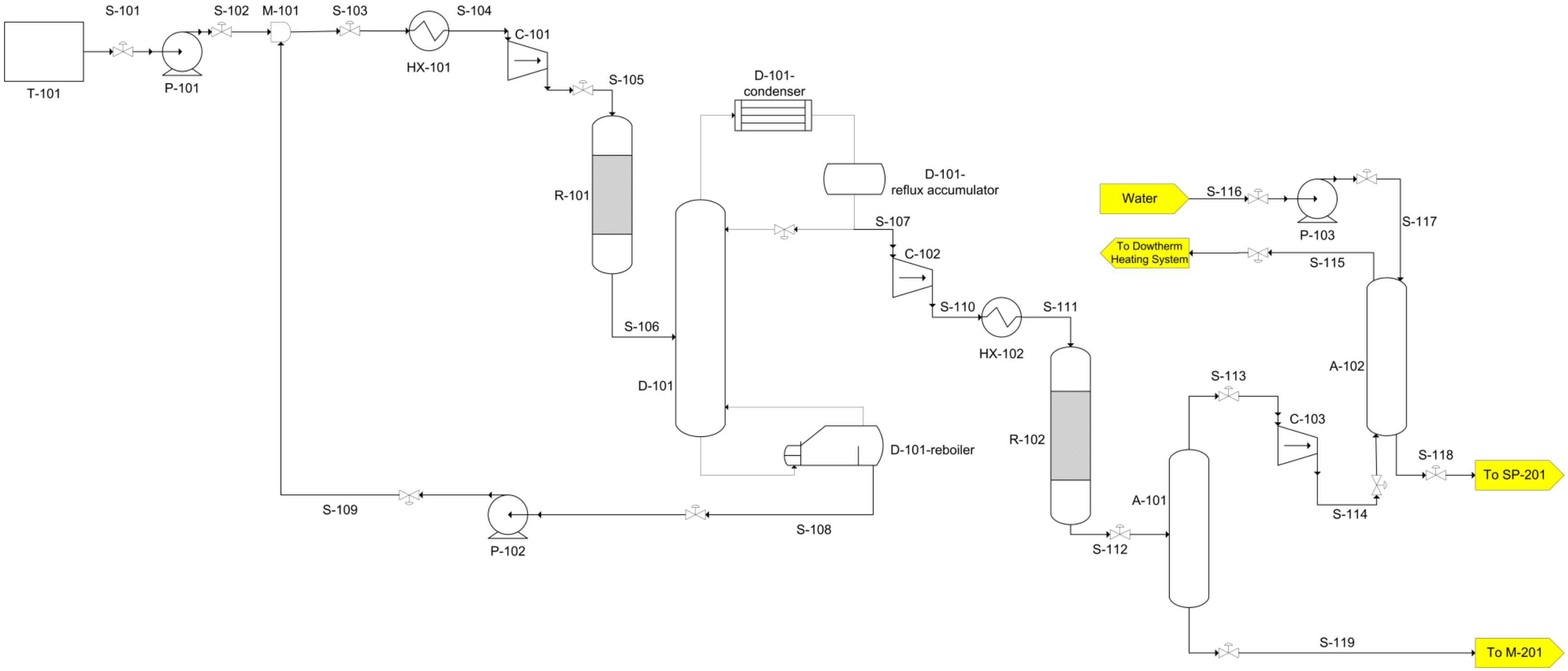
The plant designed in this report will produce 3,452 lb/hr of niacinamide at 97.7% by weight purity, targeting the animal nutrition industry as our primary consumer. This targeted output is intended to be competitive with Lonza and Jubilant but will not flood the market.

V. PROCESS DESIGN

A. PROCESS FLOW DIAGRAM AND MATERIAL BALANCES

Outlined below are the overall mass balance and stream properties. On the reactor-side of the process only preliminary mass balances were performed since separation mass balances were calculated using ASPEN simulations later in the design process. Microsoft EXCEL was used to make sure that the mass balanced with the reactions and side products that were made in the overall reaction train. This EXCEL sheet can be seen in Appendix C.

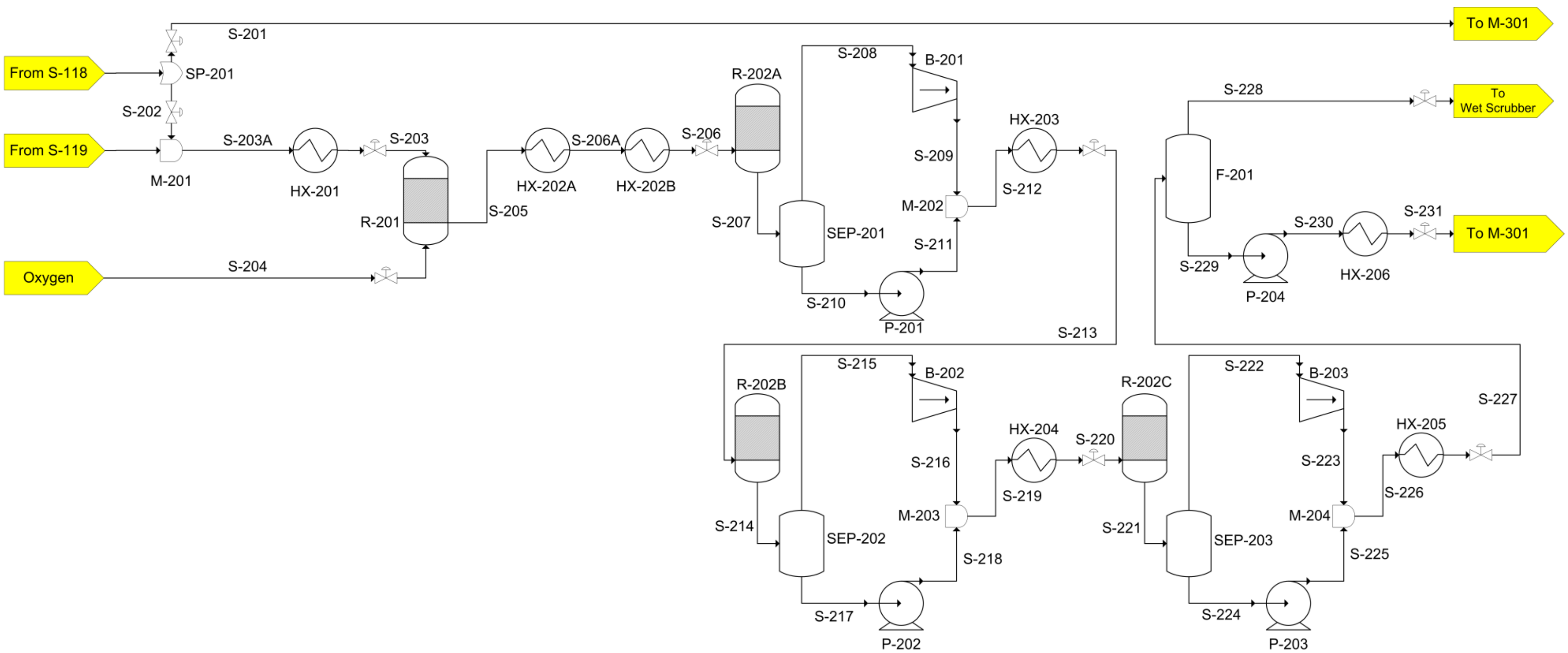
Block (100)


S-101
S-102
M-101
S-103
S-104
C-101
T-101
P-101
HX-101
S-105
D-101-
condenser
R-101
D-101-
reflux accumulator
S-107
C-102
Water
S-116
P-103
S-117
To Dowtherm
Heating System
S-115
S-106
S-110
S-111
HX-102
D-101
A-102
S-113
C-103
D-101-reboiler
R-102
S-118
To SP-201
A-101
S-114
S-109
S-108
P-102
S-112
S-119
To M-201

Block 100			Flow Rate (lb/hr)									
Name	**Formula**	**MW(lb/lb_{mol})**	**S-101**	**S-102**	**S-103**	**S-104**	**S-105**	**S-106**	**S-107**	**S-108**	**S-109**	**S-110**
Oxygen	O_2	32	0	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0	0
Ammonia	NH_3	17	0	0	2.00E-18	2.00E-18	2.00E-18	484.6719	484.6719	2.00E-18	2.00E-18	484.6719
Water	H_2O	18	0	0	0	0	0	0	0	0	0	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0	0
Niacinamide	$C_6H_6N_2O$	122.1	0	0	0	0	0	0	0	0	0	0
Methylpentanediamine	$C_6H_{16}N_2$	116.2	3306.93	3306.93	3340.33	3340.33	3340.33	33.40	0.00	33.40	33.40	0.00
Methylpiperidine	$C_6H_{13}N$	99.2	0	0	3.13E-03	3.13E-03	3.13E-03	2822.2775	2822.2744	3.13E-03	3.13E-03	2822.2744
3-Methylpyridine	C_6H_7N	93.1	0	0	0	0	0	0	0	0	0	0
3-Cyanopyridine	$C_6H_4N_2$	104.1	0	0	0	0	0	0	0	0	0	0
		Total Mass Flow (lb/hr)	**3306.93**	**3306.93**	**3340.34**	**3340.34**	**3340.34**	**3340.35**	**3306.95**	**33.40**	**33.40**	**3306.95**
		Temperature (F)	77	77.373	81.1415	527	560.2087	581	266.2846	402.3192	402.6851	393.1779
		Pressure (psia)	14.5038	43.5113	43.5113	33.5113	72.5189	71.6486	14.6959	20.5459	43.5113	72.5189
		Vapor Fraction	0	0	0	1	1	1	1	1.23E-08	0	1
		Liquid Fraction	1	1	1	0	0	0	0	1	1	0
		Enthalpy (BTU/hr)	-2.03E+06	-2.03E+06	-2.05E+06	-5.79E+05	-5.23E+05	-9.75E+05	-1.50E+06	-1.38E+04	-1.38E+04	-1.31E+06

Block 100 (cont)			Flow Rate (lb/hr)								
Name	**Formula**	**MW(lb/lb_{mol})**	**S-111**	**S-112**	**S-113**	**S-114**	**S-115**	**S-116**	**S-117**	**S-118**	**S-119**
Oxygen	O_2	32	0	0	0	0	0	0	0	0	0
Hydrogen	H_2	2	0	170.3884	170.3884	170.3884	170.3884	0	0	3.04E-14	1.55E-13
Nitrogen	N_2	28	0	0	0	0	0	0	0	0	0
Ammonia	NH_3	17	484.6719	484.6719	484.6719	484.6719	4.2846	0	0	480.3873	1.83E-06
Water	H_2O	18	0	0	0	0	8.94E-10	1200	1200	1200	0
Carbon Dioxide	CO_2	44	0	0	0	0	0	0	0	0	0
Niacinamide	$C_6H_6N_2O$	122.1	0	0	0	0	0	0	0	0	0
Methylpentanediamine	$C_6H_{16}N_2$	116.2	3.63E-03	3.63E-03	3.69E-17	3.69E-17	0	0	0	0	3.63E-03
Methylpiperidine	$C_6H_{13}N$	99.2	2822.2744	28.2227	1.47E-04	1.47E-04	3.09E-06	0	0	1.44E-04	28.2226
3-Methylpyridine	C_6H_7N	93.1	0	2623.8311	1.4148	1.4148	7.03E-06	0	0	1.4148	2622.4163
3-Cyanopyridine	$C_6H_4N_2$	104.1	0	0	0	0	0	0	0	0	0
		Total Mass Flow (lb/hr)	**3306.95**	**3307.12**	**656.48**	**656.48**	**174.67**	**1200.00**	**1200.00**	**1681.80**	**2650.64**
		Temperature (F)	554	554	5.9902	313.672	-117.8784	90	90.9526	224.717	366.2599
		Pressure (psia)	62.5189	42.2136	40	170	170	15	170	170	40
		Vapor Fraction	1	1	1	1	1	0	0	5.12E-06	4.44E-07
		Liquid Fraction	0	0	0	0	0	1	1	1	1
		Enthalpy (BTU/hr)	-1.02E+06	1.58E+06	-6.19E+05	-3.61E+05	-1.17E+05	-8.26E+06	-8.26E+06	-8.91E+06	1.08E+06

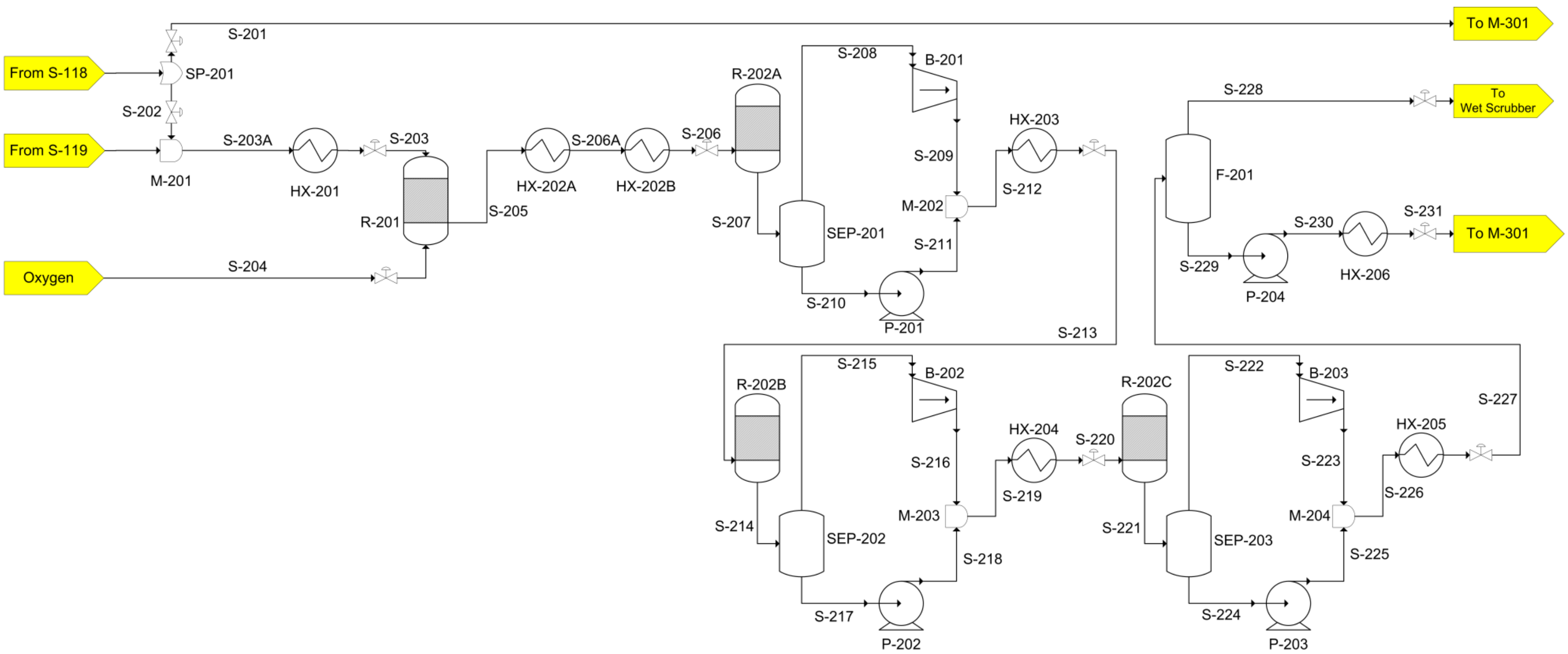
Block (200)


S-201
To M-301
From S-118
SP-201
S-208
B-201
R-202A
S-228
To Wet Scrubber
S-202
HX-203
From S-119
S-203A
S-203
S-206A
S-206
S-209
F-201
M-201
HX-201
HX-202A
HX-202B
S-212
M-202
S-230
S-231
To M-301
R-201
S-205
S-207
SEP-201
S-211
Oxygen
S-204
S-229
HX-206
P-204
S-210
P-201
S-213
S-215
B-202
S-222
B-203
R-202B
R-202C
S-227
HX-204
S-220
HX-205
S-216
S-223
S-219
S-226
M-203
M-204
S-214
S-221
SEP-202
SEP-203
S-218
S-225
S-217
S-224
P-202
P-203

Block 200			Flow Rate (lb/hr)									
Name	**Formula**	**MW(lb/lb$_{mol}$)**	**S-201**	**S-202**	**S-203**	**S-203A**	**S-204**	**S-205**	**S-206**	**S-206A**	**S-207**	**S-208**
Oxygen	O_2	32	0	0	0	0	1481.4509	135.6763	135.6763	135.6763	135.6763	135.42
Hydrogen	H_2	2	3.34E-16	3.00E-14	1.85E-13	1.85E-13	0	0	0	0	0	0
Nitrogen	N_2	28	0	0	0	0	0	0.3946	0.3946	0.3946	0.3946	0.3945
Ammonia	NH_3	17	5.2843	475.103	475.1031	475.1031	0	7.89E-02	7.89E-02	7.89E-02	7.89E-02	4.25E-03
Water	H_2O	18	13.2	1186.8	1186.8	1186.8	0	2696.0476	2696.0476	2696.0476	2198.5821	2.5583
Carbon Dioxide	CO_2	44	0	0	0	0	0	7.4396	7.4396	7.4396	7.4396	7.1777
Niacinamide	$C_6H_6N_2O$	122.1	0	0	0	0	0	0	0	0	3372.1643	2.08E-04
Methylpentanediamine	$C_6H_{16}N_2$	116.2	0	0	3.63E-03	3.63E-03	0	3.63E-03	3.63E-03	3.63E-03	3.63E-03	1.56E-04
Methylpiperidine	$C_6H_{13}N$	99.2	1.58E-06	1.42E-04	28.2227	28.2227	0	28.2227	28.2227	28.2227	28.2227	2.0383
3-Methylpyridine	C_6H_7N	93.1	1.56E-02	1.3993	2623.8156	2623.8156	0	23.6143	23.6143	23.6143	23.6143	0.7393
3-Cyanopyridine	$C_6H_4N_2$	104.1	0	0	0	0	0	2903.918	2903.918	2903.918	29.0392	0.1032
		Total Mass Flow (lb/hr)	**18.50**	**1663.30**	**4313.95**	**4313.95**	**1481.45**	**5795.40**	**5795.40**	**5795.40**	**5795.22**	**148.44**
		Temperature (F)	224.717	224.717	626	158.8554	77	626	77	100	77	77
		Pressure (psia)	170	170	30	40	39.4503	29.1298	19.1298	24.1298	14.7298	14.7298
		Vapor Fraction	5.12E-06	5.1152E-06	1	0.060995	1	1	0.024904	0.025426	0.029574	1
		Liquid Fraction	1	1	0	0.939	0	0	0.9751	0.9746	0.9704	0
		Enthalpy (BTU/hr)	-9.80E+04	-8.81E+06	-5.13E+06	-7.73E+06	-4.45E+02	-1.10E+07	-1.55E+06	-1.54E+07	-1.66E+07	-4.28E+04

Block 200 (cont)			Flow Rate (lb/hr)									
Name	**Formula**	**MW(lb/lb$_{mol}$)**	**S-209**	**S-210**	**S-211**	**S-212**	**S-213**	**S-214**	**S-215**	**S-216**	**S-217**	**S-218**
Oxygen	O_2	32	135.42	0.2563	0.2563	135.6763	135.6763	135.6763	135.411	135.411	0.2654	0.2654
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0.3945	8.58E-05	8.58E-05	0.3946	0.3946	0.3946	0.3945	0.3945	8.88E-05	8.88E-05
Ammonia	NH_3	17	4.25E-03	7.47E-02	7.47E-02	7.89E-02	7.89E-02	7.89E-02	4.12E-03	4.12E-03	7.48E-02	7.48E-02
Water	H_2O	18	2.5583	2196.0238	2196.0238	2198.5821	2198.5821	2198.5821	2.4717	2.4717	2196.1104	2196.1104
Carbon Dioxide	CO_2	44	7.1777	0.2619	0.2619	7.4396	7.4396	7.4396	7.1688	7.1688	0.2708	0.2708
Niacinamide	$C_6H_6N_2O$	122.1	2.08E-04	3372.1641	3372.1641	3372.1643	3372.1643	3372.1643	2.01E-04	2.01E-04	3372.1641	3372.1641
Methylpentanediamine	$C_6H_{16}N_2$	116.2	1.56E-04	3.47E-03	3.47E-03	3.63E-03	3.63E-03	3.63E-03	1.51E-04	1.51E-04	3.47E-03	3.47E-03
Methylpiperidine	$C_6H_{13}N$	99.2	2.0383	26.1844	26.1844	28.2227	28.2227	28.2227	1.9747	1.9747	26.2481	26.2481
3-Methylpyridine	C_6H_7N	93.1	0.7393	22.875	22.875	23.6143	23.6143	23.6143	0.7153	0.7153	22.8991	22.8991
3-Cyanopyridine	$C_6H_4N_2$	104.1	0.1032	28.936	28.936	29.0392	29.0392	29.0392	9.98E-02	9.98E-02	28.9394	28.9394
		Total Mass Flow (lb/hr)	**148.44**	**5646.78**	**5646.78**	**5795.22**	**5795.22**	**5795.22**	**148.24**	**148.24**	**5646.98**	**5646.98**
		Temperature (F)	249.416	77	77.1252	78.9689	77	77	77	228.908	77	77.1252
		Pressure (psia)	31.8503	14.7298	29.7298	29.7298	19.7298	15.2298	15.2298	30.2298	15.2298	30.2298
		Vapor Fraction	1	0	0	0.028952	0.029258	0.029534	1	1	0	0
		Liquid Fraction	0	1	1	0.971	0.9707	0.9705	0	0	1	1
		Enthalpy (BTU/hr)	-3.69E+04	-1.66E+07	-1.66E+07	-1.66E+07	-1.66E+07	-1.66E+07	-4.22E+04	-3.71E+04	-1.66E+07	-1.66E+07

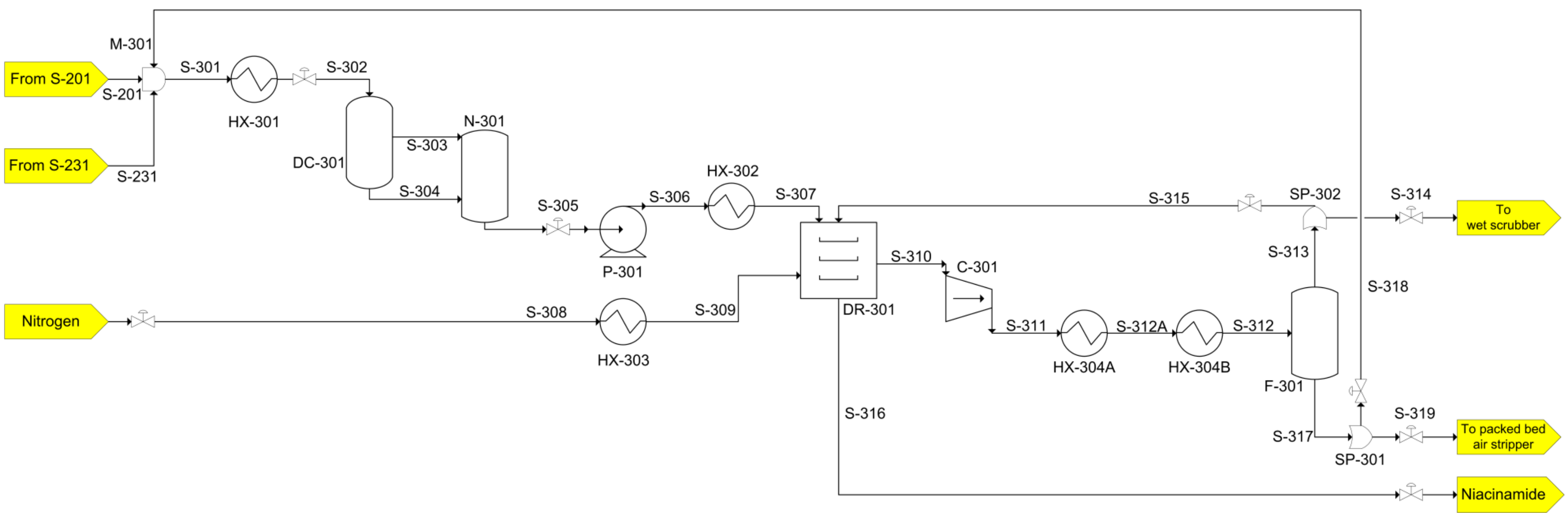
Block (200) (Streams continued)



Block 200 (cont)			Flow Rate (lb/hr)									
Name	Formula	MW(lb/lb$_{mol}$)	S-219	S-220	S-221	S-222	S-223	S-224	S-225	S-226	S-227	S-228
Oxygen	O_2	32	135.6763	135.6763	135.6763	135.4019	135.4019	0.2744	0.2744	135.6763	135.6763	135.4641
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	0.3946	0.3946	0.3946	0.3945	0.3945	9.18E-05	9.18E-05	0.3946	0.3946	0.3946
Ammonia	NH_3	17	7.89E-02	7.89E-02	7.89E-02	3.99E-03	3.99E-03	7.49E-02	7.49E-02	7.89E-02	7.89E-02	1.32E-03
Water	H_2O	18	2198.5821	2198.5821	2198.5821	2.3908	2.3908	2196.1913	2196.1913	2198.5821	2198.5821	0.4615
Carbon Dioxide	CO_2	44	7.4396	7.4396	7.4396	7.1599	7.1599	0.2797	0.2797	7.4396	7.4396	7.0928
Niacinamide	$C_6H_6N_2O$	122.1	3372.1643	3372.1643	3372.1643	1.95E-04	1.95E-04	3372.1641	3372.1641	3372.1643	3372.1643	1.17E-05
Methylpentanediamine	$C_6H_{16}N_2$	116.2	3.63E-03	3.63E-03	3.63E-03	1.46E-04	1.46E-04	3.48E-03	3.48E-03	3.63E-03	3.63E-03	6.52E-05
Methylpiperidine	$C_6H_{13}N$	99.2	28.2227	28.2227	28.2227	1.915	1.915	26.3078	26.3078	28.2227	28.2227	1.1116
3-Methylpyridine	C_6H_7N	93.1	23.6143	23.6143	23.6143	0.6927	0.6927	22.9216	22.9216	23.6143	23.6143	0.3275
3-Cyanopyridine	$C_6H_4N_2$	104.1	29.0392	29.0392	29.0392	9.65E-02	9.65E-02	28.9426	28.9426	29.0392	29.0392	3.31E-02
Total Mass Flow (lb/hr)			**5795.22**	**5795.22**	**5795.22**	**148.06**	**148.06**	**5647.16**	**5647.16**	**5795.22**	**5795.22**	**144.89**
		Temperature (F)	78.7705	77	77	77	275.3011	77	77.2505	79.3753	32	32
		Pressure (psia)	30.2298	20.2298	15.7298	15.7298	37.7298	15.7298	45.7298	37.7298	27.7298	15
		Vapor Fraction	0.028936	0.029234	0.029496	1	1	0	0	0.028787	0.028529	1
		Liquid Fraction	0.9711	0.9708	0.9705	0	0	1	1	0.9712	0.9715	0
		Enthalpy (BTU/hr)	-1.66E+07	-1.66E+07	-1.66E+07	-4.17E+04	-3.50E+04	-1.66E+07	-1.66E+07	-1.66E+07	-1.68E+07	-3.16E+04

Block 200 (cont)			Flow Rate (lb/hr)		
Name	Formula	MW(lb/lb$_{mol}$)	S-229	S-230	S-231
Oxygen	O_2	32	0.2122	0.2122	0.2122
Hydrogen	H_2	2	0	0	0
Nitrogen	N_2	28	5.32E-05	5.32E-05	5.32E-05
Ammonia	NH_3	17	7.76E-02	7.76E-02	7.76E-02
Water	H_2O	18	2198.1206	2198.1206	2198.1206
Carbon Dioxide	CO_2	44	0.3468	0.3468	0.3468
Niacinamide	$C_6H_6N_2O$	122.1	3372.1643	3372.1643	3372.1643
Methylpentanediamine	$C_6H_{16}N_2$	116.2	3.56E-03	3.56E-03	3.56E-03
Methylpiperidine	$C_6H_{13}N$	99.2	27.1112	27.1112	27.1112
3-Methylpyridine	C_6H_7N	93.1	23.2869	23.2869	23.2869
3-Cyanopyridine	$C_6H_4N_2$	104.1	29.0061	29.0061	29.0061
Total Mass Flow (lb/hr)			**5650.33**	**5650.33**	**5650.33**
		Temperature (F)	32	32.2422	90
		Pressure (psia)	15	45	35
		Vapor Fraction	0	0	0
		Liquid Fraction	1	1	1
		Enthalpy (BTU/hr)	-1.68E+07	-1.68E+07	-1.65E+07

Block (300)



M-301
From S-201
S-201
S-301
HX-301
S-302
From S-231
S-231
DC-301
S-303
N-301
S-304
S-305
P-301
S-306
HX-302
S-307
DR-301
S-310
C-301
S-311
HX-304A
S-312A
HX-304B
S-312
F-301
S-313
SP-302
S-315
S-314
To wet scrubber
S-318
S-317
SP-301
S-319
To packed bed air stripper
S-316
Niacinamide
Nitrogen
S-308
HX-303
S-309

Block 300			Flow Rate (lb/hr)									
Name	**Formula**	**MW(lb/lb$_{mol}$)**	**S-301**	**S-302**	**S-304**	**S-305**	**S-306**	**S-307**	**S-308**	**S-309**	**S-310**	**S-311**
Oxygen	O_2	32	0.2129	0.2129	0.2129	0.2129	0.2129	0.2129	0	0	2.1222	2.1222
Hydrogen	H_2	2	3.34E-16	3.34E-16	3.34E-16	0	0	0	0	0	0	0
Nitrogen	N_2	28	2.09E-03	2.09E-03	2.09E-03	2.09E-03	2.09E-03	2.09E-03	30.8796	30.8796	308.7963	308.7963
Ammonia	NH_3	17	53.5941	53.5941	53.5941	53.5941	53.5941	53.5941	0	0	53.6188	53.6188
Water	H_2O	18	2.21E+04	2.21E+04	2.21E+04	2.21E+04	2.21E+04	2.21E+04	0	0	2.21E+04	2.21E+04
Carbon Dioxide	CO_2	44	0.3659	0.3659	0.3659	0.3659	0.3659	0.3659	0	0	3.4681	3.4681
Niacinamide	$C_6H_6N_2O$	122.1	3372.1643	3372.1643	3372.1643	3372.1643	3372.1643	3372.1643	0	0	0	0
Methylpentanediamine	$C_6H_{16}N_2$	116.2	3.56E-03	3.56E-03	3.56E-03	3.56E-03	3.56E-03	3.56E-03	0	0	0	0
Methylpiperidine	$C_6H_{13}N$	99.2	27.1112	27.1112	27.1112	27.1112	27.1112	27.1112	0	0	0	0
3-Methylpyridine	C_6H_7N	93.1	23.3024	23.3024	23.3024	23.3024	23.3024	23.3024	0	0	0	0
3-Cyanopyridine	$C_6H_4N_2$	104.1	29.0061	29.0061	29.0061	29.0061	29.0061	29.0061	0	0	0	0
Total Mass Flow (lb/hr)			**25618.76**	**25618.76**	**25618.76**	**25618.76**	**25618.76**	**25618.76**	**30.88**	**30.88**	**22481.01**	**22481.01**
		Temperature (F)	30.9724	77	77.0265	77	76.9392	392	77	392	387.1028	887.2012
		Pressure (psia)	35	25	20	15	39.9465	29.9465	29.5007	19.5007	14.5007	68.0082
		Vapor Fraction	0.00034792	0.00026201	0.00030069	0.00035328	0	1	1	1	1	1
		Liquid Fraction	0.9997	0.9997	0.9997	0.9996	1	0	0	0	0	0
		Enthalpy (BTU/hr)	-1.55E+08	-1.54E+08	-1.54E+08	-1.54E+08	-1.54E+08	-1.25E+08	-5.9364	2425.2806	-0.3685	-1.19E+08

Block 300 (cont)			Flow Rate (lb/hr)								
Name	**Formula**	**MW(lb/lb$_{mol}$)**	**S-312**	**S-312A**	**S-313**	**S-314**	**S-315**	**S-316**	**S-317**	**S-318**	**S-319**
Oxygen	O_2	32	2.1222	2.1222	2.1214	0.2121	1.9093	0	7.50E-04	6.75E-04	7.50E-05
Hydrogen	H_2	2	0	0	0	0	0	0	0	0	0
Nitrogen	N_2	28	308.7963	308.7963	308.794	30.8794	277.9146	0	2.27E-03	2.04E-03	2.27E-04
Ammonia	NH_3	17	53.6188	53.6188	2.73E-02	2.73E-03	2.46E-02	0	53.5914	48.2323	5.3591
Water	H_2O	18	2.21E+04	2.21E+04	0.2025	2.03E-02	0.1823	0	2.21E+04	1.99E+04	2211.3003
Carbon Dioxide	CO_2	44	3.4681	3.4681	3.4469	0.3447	3.1022	0	2.12E-02	1.91E-02	2.12E-03
Niacinamide	$C_6H_6N_2O$	122.1	0	0	0	0	0	3372.1643	0	0	0
Methylpentanediamine	$C_6H_{16}N_2$	116.2	0	0	0	0	0	3.56E-03	0	0	0
Methylpiperidine	$C_6H_{13}N$	99.2	0	0	0	0	0	27.1112	0	0	0
3-Methylpyridine	C_6H_7N	93.1	0	0	0	0	0	23.3024	0	0	0
3-Cyanopyridine	$C_6H_4N_2$	104.1	0	0	0	0	0	29.0061	0	0	0
Total Mass Flow (lb/hr)			**22481.01**	**22481.01**	**314.59**	**31.46**	**283.13**	**3451.59**	**22166.62**	**19950.25**	**2216.66**
		Temperature (F)	32	100	32	31.6692	31.6692	387.1028	32	32.0274	32.0274
		Pressure (psia)	58.0082	63.0082	58.0082	48.0082	48.0082	14.5007	58.0082	48.0082	48.0082
		Vapor Fraction	0.009	0.0091	1	1	1	0	0	1	1
		Liquid Fraction	0.991	0.9909	0	0	0	1	1	0	0
		Enthalpy (BTU/hr)	-1.54E+08	-1.52E+08	-1.81E+04	-1810.8	-1.63E+04	-1.17E+06	-1.54E+08	-1.38E+08	-1.54E+07

B. PROCESS DESCRIPTION

The proposed process is separated into three blocks. The first block (Block 100) involves the reaction train in which MPDA is converted to PIC. The second block (Block 200) involves the reaction train in which PIC is converted to the desired product: niacinamide. The last block (Block 300) includes the purification and separation of the niacinamide to give the desired end product.

Block (100): Reaction Train 1—MPDA to PIC

Summary

S-101 is the input for the process containing liquid MPDA. This stream undergoes a pressure increase and is then passed through a heat exchanger where the MPDA is vaporized. The MPDA is then compressed and passed through the first reactor. Reactor 1 converts the MPDA to methylpiperidine with a byproduct of ammonia. More information about reactor 1 can be found in the Reactor Design section. The distillation column that follows separates out the unreacted MPDA to be recycled back into the first reactor while the remaining organic compounds and the ammonia continue through the process. The stream is compressed again and fed into Reactor 2 which converts the methylpiperidine to 3-picoline with a byproduct of hydrogen gas.

The next vessel is an absorbing column that closely resembles a distillation tower. The distillate product is ammonia and hydrogen, which is fed into a second absorbing column where ammonia is absorbed into the incoming process water in stream S-116 and the hydrogen leaves the absorbing column via stream S-115. This hydrogen would then be used for the fuel required by the Dowtherm process illustrated later, which is burned in excess air. The remaining ammonia and water stream, S-118, is fed into a splitter to be fed into the second block of the process.

Reactor Design

Reactor Train 1 (R-101)

The first step in the process is the cyclization/deamination of MPDA to form MPI and ammonia as a byproduct. This takes place through a tubular reactor at temperatures and pressures in the range of 572 – 752°F and 0 – 145 psia respectively over activated Al_2O_3/SiO_2 catalysts or zeolites. As the availability of information regarding the kinetics of the reaction is greatly limited, the initial basis of the reactor's design was based on the patent by Lonza (Heveling et al., 1998) in which a range of reaction conditions and their corresponding yields and conversions for a bench-scale set-up were documented. The optimal conditions that gave the highest conversion for the first reaction were found to occur at 581°F at a pressure of 72.5 psia with a mass hourly space velocity (MHSV) of 4.2 lb/lb-hr over HZSM-5 catalysts. The composition of HZSM-5 catalysts to be used is 54.5% of pentasil (Si/Al = 18) + 45.5% of binder.

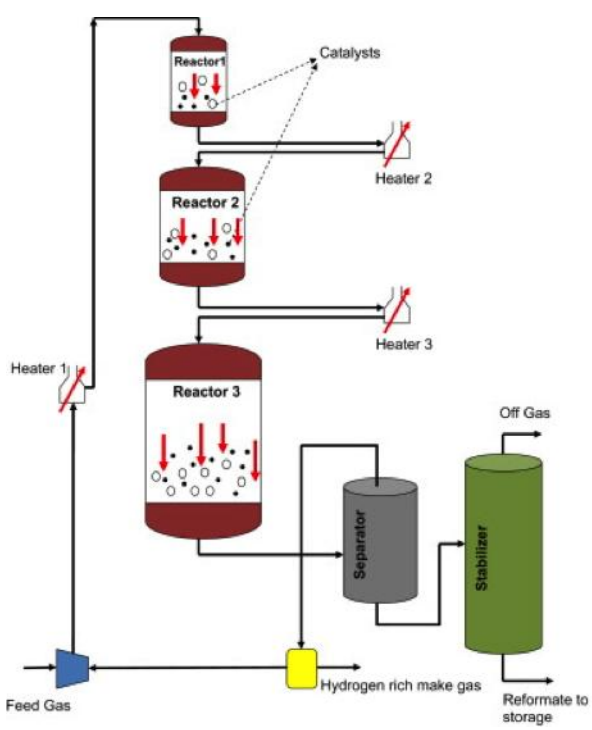


Figure 3. Schematic of the conventional catalytic naphtha reforming process. Source: Iranshahi, et al., 2009

For the design of Reactor Train 1, similar reactions were researched to find the best reactor for the unit. In drawing similarities between the first reaction in the train and that of commercial naphtha reforming (Figure 3) - where straight-chained organics are converted into more useful products, usually cyclic materials, (Fundamentals of Industrial Catalytic Processes) - it was found that a semi-regenerative unit containing the catalyst outlined by Lonza may provide the best conversion. Therefore, Reactor Train 1 is designed as a tubular reactor operating at 581°F at a pressure of 72.5 psia with a mass hourly space velocity (MHSV) of 0.6 lb/lb-hr over HZSM-5 catalysts. The percentage conversion given in the patent for MPDA to MPI is 99.6%. The reaction is optimal at a temperature of 581°F, but the reaction is exothermic; therefore, the initial feed is sent through four reactors, each in increasing size, with a cooling unit between each reactor to keep a relatively constant temperature of 581°F. This allows the stream to stay within the range of optimal catalytic selectivity, overall conversion, and minimal catalyst degradation. By using this design, a similar conversion to that of what was expressed in the Lonza process with tubular reactors can be accomplished. Within each of these reactors, H-ZSM-5 would be used as the heterogeneous catalyst.

Reactor Sizing

Approximately 3,340 lb/hr of MPDA vapor at 560°F and 72.5 psia is fed into the first reactor of Reactor Train 1. When the MPDA vapor enters the first reactor, it reacts upon contact with the catalyst, increasing the temperature. It should then pass through the cooling unit before entering the next reactor of the reactor train, decreasing the reactor temperature. The resulting temperature profile would then have an approximate saw-tooth appearance. Overall the average temperature is approximately 581°F.

Amount of Catalyst

The volume of catalyst required was calculated via scaling up from the patent to determine the amount needed to convert 3,340 lb/hr of MPDA. With a MHSV of 0.6 lb/lb-hr, 5,600 lb of HZSM-5 catalyst were required for the entire reactor train. Assuming a catalyst density of 50 lb/ft^3 and a void fraction of 0.5, the total volume of catalysts required would then be 224 ft^3. The total price of the catalyst is $3,810. Please reference page 234 for Sample Calculations.

Tube Dimensions and Number of Tubes

When choosing the tube dimensions, the main considerations were to maximize heat transfer across the tubes. This consideration advocated for a small tube diameter. Another consideration made was to minimize the difference between internal and external diameters of the tube to allow for more efficient heat conduction across the tube material. As such the catalyst was modeled in a ring form with a thickness of 1 inch on each side. With a required catalyst volume of 224 ft^3, this gave the overall tube length of 10,270 ft. A nominal pipe size of 6 inches was chosen for the tube. To account for a more manageable reactor length, fifteen tubes will be used, giving the length of one tube to be 685 ft, with the catalyst support accounted for. Using 15 tubes, the volumetric flow rate through one tube then becomes 1,010 ft^3/hr, thereby giving a superficial velocity of 3.6 ft/s through one tube, a reasonable velocity for vapor through a tube to react. At these dimensions, the Reynolds number for flow through the tubes is small enough that the reactants can approximate plug-flow conditions. Since the overall catalyst requirement is 224 ft^3, the reactor length ratio for each of the four reactors should be, in increasing order, 68: 103: 171: 342 ft. In addition, a recycled loop may be added to the overall system to increase the percent conversion of MPDA added into the system. In this manner, the reactor would be designed as a semi-regenerative reactor unit with four reactors and a large cooling unit integrated into the process to cool the reaction feeds since the overall reaction is exothermic (Askari, A., et al., 2012).

Pressure Drop

To estimate the pressure drop across the reactor, the Darcy–Weisbach equation was used. Operating at 72.5 psi at the above dimensions, the pressure drop across the tubes was 0.87 psi. The pressure is relatively small since it is a homogeneous tubular reactor. The pressure remains relatively constant throughout the process; therefore, this reaction train can operate at the specified 72.5 psia without significant pressure drop.

Heat Transfer Considerations

With a heat duty of -452,100 Btu/hr, it was determined that 15,118 lb/hr of cooling water was required as a cooling utility. Based on the volumetric ratios of the reactors, the ratio of cooling water required for each cooling section after each reactor is 1,505: 2,269: 3,781: 7,563 lb/hr. The overall heat transfer coefficient is set at 60 Btu/lb-hr-°F as per consultants' (Mr. Wismer and Mr. Kolesar) suggestion.

Reactor Train 2 (R-102)

The second step in the process is the endothermic dehydrogenation of MPI to PIC, producing hydrogen as a byproduct. According to Lonza's patent, the second reaction preferably takes place in a fixed-bed reactor filled with noble metals as catalysts, such as Pd or Pt, on a support at 428 – 752°F and pressures of 0 – 145 psia. Again, based on the patent by Lonza (Heveling et al., 1998), the optimal conditions were found to occur at 554°F at atmospheric pressure with 0.44 lb/lb-hr MHSV over 1% Pd-SiO_2/Al_2O_3 catalysts.

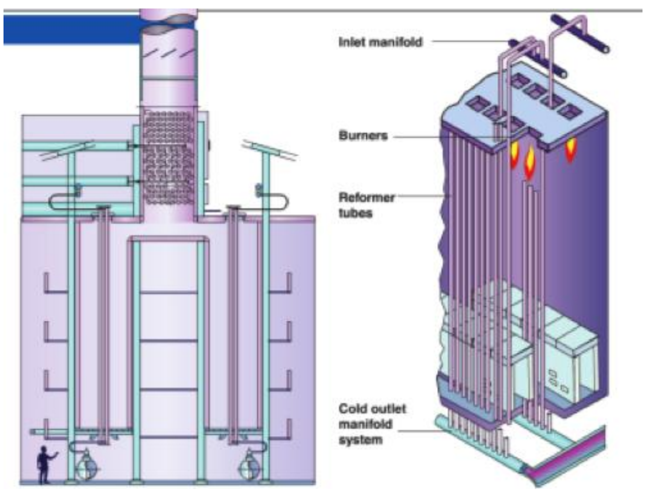


Figure 4. Reformer Furnace Design. Source: "Hydrogen Production by Steam Reforming", Ray Elshout, Chemical Engineering, May 2010

Reactor 2 is also designed using a reaction similar to one already present in commercial processing. In the Fischer-Tropsch process, which converts hydrogen and carbon monoxide to hydrocarbons, multi-tubular reactors are used to aid in the steam reforming piece of Fischer-Tropsch (Figure 4)(Elshout, R., 2010). In steam reforming, feed is run through a series of packed bed reactor tubes, which are heated by a fuel source or in this case, a Dowtherm heated material. The reaction tubes are arranged such that the reactants are fed into the reactor at a much higher temperature than the exit so that the reaction can proceed throughout the entire tube length. For a typical process, approximately 2,000 tubes or more can be placed into one furnace. Each tube has a typical diameter of between 2.8 and 5.1 inches with a length of 39.4 ft. Residence times for these reactors would be 5 seconds per each tube. With this short residence time, pressure drop across the reactor is minimized and the reactor volume itself can also be decreased. (Bartholomew & Farrauto, 2005).

Amount of Catalyst

From S-111, approximately 3,310 lb/hr of material at 554°F at 40 psia is fed into Reactor 2 at 9,680 ft^3/hr. Stream S-111 primarily consists of approximately 0.15 mass% of ammonia and 0.85 mass% of MPI. From the patent, the volume of catalyst required was calculated via scaling up to determine the amount needed to convert 2,822 lb/hr of MPI. With a MHSV of 0.44 lb/lb-hr, 6,410 lb of 1% Pd-SiO_2/Al_2O_3 catalysts were required for the entire reactor train. Assuming a weighted catalyst density of 211 lb/ft^3 and a void fraction of 0.5, the total volume of catalysts required would then be 60 ft^3. The total price of the catalyst is $ 783,300. Please reference page 236 for Sample Calculations.

Reactor Sizing

Based on the volume of catalyst required, the conventional Fischer-Tropsch reactor would need to be scaled down to the following specifications: 40 tubes with a tube length of 20 ft and a diameter of 4 inches.

Pressure Drop

To estimate the pressure drop across the reactor, the Ergun equation for packed bed was used. The pressure drop across the 20-feet tubes was 4.5 psi. This pressure drop across the tubes is an industry practice upper bound.

Heat Transfer Requirements

With a heat duty of 2.602 MMBtu/hr, 10,408 lb/hr of Dowtherm A will be used as the heat transfer fluid used to supply the energy required to attain the operating temperature conditions. The overall heat transfer coefficient is set at 60 Btu/lb-hr-°F as per consultants' (Mr. Wismer and Mr. Kolesar) suggestion.

Process Modeling

To model the first block of the process, ASPEN V 7.3.1 was used. However, due to the complexity of the process, some simplifications and assumptions were made to use ASPEN to simulate the overall process. It is known that a separation column was used in Lonza's process to separate and divert the unreacted MPDA to be recycled back to the first reactor (ICIS.com, 1999). It is assumed that this separation unit was a distillation column. In ASPEN, this distillation column was modeled using RADFRAC, which did a relatively good job of calculating the energy and tray requirements for the separation. Additionally, there were two absorbers added to the process to help separate hydrogen from the system after the second reactor; by removing this stream, the hydrogen can be fed to a Dowtherm system as fuel, whereas the remainder of the units in the process could also be decreased in size due to the absence of hydrogen. In ASPEN, these two absorbers were modeled using the ABSRB1 and ABSRB2 subroutine under the RADFRAC unit, respectively. The second absorbing column, A-102, was used with water as the absorbing agent because ammonia dissolves readily in this solvent, leaving hydrogen in the other stream to be used later as a fuel.

Block (200): Reaction Train 2—PIC to Niacinamide

Summary

The second block was modeled in ASPEN V 7.3.1. Input into this block is a fraction of the ammonia and water mixture that was taken off of A-102. The stoichiometric ratio of ammonia was taken from the splitter to be heated and then added to the third reactor, R-201. The other stream heading to the reactor consists of 3-picoline and the unreacted methylpiperidine as well as trace amounts of other organics. This stream, S-119, is added to M-201 and mixed with the ammonia water mixture, heated, and fed to R-201. Stream S-204 is the feed stream of oxygen required to react with 3-picoline in the reactor. In R-201, 3-picoline reacts with oxygen and converts to 3-cyanopyridine with a byproduct of water. In addition, this reactor models the side reactions that would occur in the presence of oxygen; these side reactions take the organic molecules present in the reactors and convert them to nitrogen, carbon dioxide, and water. The stream then continues to a two-stage heat exchanger to cool to more moderate operating conditions needed for the biocatalyst reactors. After this stream is cooled, it enters a CSTR reactor that contains the biocatalyst necessary to react 3-cyanopyridine with water to make niacinamide. The vapor and liquid streams from this reactor are moved by blowers and compressors, respectively, to the next reactor. This occurs for three CSTRs in series; three CSTRs in series not only increase the conversion but also allows for a longer residence time in each of the reactors.

After the final CSTR, stream S-226 is cooled down to help separate the vapor products present in the stream before the organic trace materials and the niacinamide continues to the third block in the process. S-228, the waste stream from the flash vessel, contains mostly oxygen, hydrogen, and water vapor. Some trace organics are present in this stream including CNP, PIC, and MPI. However, this stream will later be cleansed of these contaminants. Before being transferred to the third block, the stream containing mostly organics and water is heated and mixed in M-301 with the remainder of the ammonia and water mixture taken from the splitter in Block 100.

Reactor Design

Reactor Train 3

The third step in the process is the exothermic ammoxidation for the production of 3-cyanopyridines (and water as a byproduct) using ammonia and oxygen with PIC. The preferred design is that the reaction takes place at temperatures of 536 – 752°F in a multi-tubular reactor over a catalyst consisting of oxides of vanadium, titanium, zirconium, and molybdenum at atmospheric pressure (Heveling et al., 1998). Two Lonza patents (Heveling et al., 1998 and Sembaev et al., 1997) determine that the optimal conditions are at 626°F and atmospheric pressure, with catalysts consisting of V_2O_5, TiO_2, and ZrO_2 in a 1:3:8 molar ratio and MoO_3 as 1.15 w% based on V_2O_5. The molar composition of the feed into Reactor 3 is ideally PIC:O_2:NH_3 = 1:40:1.3.

Reactor 3 is designed as a multitubular reactor as used in the Fischer-Tropsch synthesis. In the same manner as Reactor 2, a steam reforming reactor design can be implemented to increase the yield of the reaction. However, instead of using the Dowtherm to heat the reaction, a cooling fluid would flow through the reactor to decrease the temperature as necessary throughout the reactor. This reactor comprises a single shell compartment with 2,000 tubes filled with catalysts in the form of rings. Each individual tube will have an internal diameter of 1.8 in and a length of 42 ft as scaled up from *Modeling of Multi-Tubular Reactors for Fischer-Tropsch Synthesis* (Jess & Kern, 2009). The overall reactor geometry is similar to that of conventional shell-and-tube type heat exchangers, but with no tube zone in the center of the reactor. The reacting gas enters at the bottom of the unit. The optimal conditions are at 626°F and atmospheric pressure, with catalysts consisting of V_2O_5, TiO_2, ZrO_2, and MoO_3.

Amount of Catalyst

From S-203, approximately 4,314 lb/hr of material at 626°F at 30 psia is fed into Reactor 3 at 47,200 ft^3/hr. Stream S-203 primarily consists of approximately 0.11 mass% of ammonia, 0.28 mass% of water, and 0.61 mass% of PIC. From the patent, the volume of catalyst required was calculated via scaling up to determine the amount needed to convert 2,624 lb/hr of PIC. With a MHSV of 5.24 lb PIC/ft^3 catalyst-hr, and assuming a void fraction of 0.5, 1,000 ft^3 of V_2O_5, TiO_2, ZrO_2, and MoO_3 catalysts were required for the entire reactor. For this volume, at the specified ratio, 90,500 lb of V_2O_5, 39,800 lb of TiO_2, 61,300 lb of ZrO_2, and 71,700 lb of MoO_3 would be required for a total of 263,300 lb of catalyst. The catalysts should be mixed well and formed into circular rings with a wall thickness of 0.4 inches that would line the inner diameter of the tubes. The total price of the catalyst is $ 1,646,000. Please refer to page 237 for Sample Calculations.

Reactor Sizing

Based on the volume of catalyst required, the conventional Fischer-Tropsch reactor would need to be scaled down to the following specifications: 2,000 tubes with a tube length of 42 ft and diameter of 1.8 in.

Pressure Drop

To estimate the pressure drop across the reactor, the Darcy–Weisbach equation was used. At the reactor dimensions, the pressure drop across the tubes was 0.87 psi. The pressure is relatively small since it is a homogeneous tubular reactor. Since the pressure remains relatively constant throughout the process; therefore, there should be no issues in significant pressure drop.

Heat Transfer Requirements

With a heat duty of -5.88 MMBtu/hr, it was determined that 196,694 lb/hr of cooling water was required as a cooling utility to attain and maintain the operating temperature conditions. The overall heat transfer coefficient is set at 60 Btu/lb-hr-°F as per consultants' (Mr. Wismer and Mr. Kolesar) suggestion.

Reactor Train 4

The fourth step in the process is the enzymatic hydrolysis of 3-cyanopyridine to niacinamide in a continuous feed batch reactor cascade comprising of 2 – 5 connected stirred reactors, catalyzed by an enzyme produced by microorganisms of the species *Rhodococcus rhodochrous* J1, which is immobilized, over temperatures of 41 – 122°F at atmospheric pressure. According to the Lonza patent (Heveling et al., 1998), the process is best carried out at ambient temperature and pressure using the species *Rhodococcus rhodochrous* J1 with the concentration of 3-cyanopyridine being 6.24 lb/ft^3. Lonza Guangzhou Fine Chemicals (Guangzhou, China) uses a series of stirred-tank multi stage batch reactors with a continuous feed of 3-cyanopyridine at concentrations of between 10–20 wt% in the direction of process flow, and counter-current feed of biocatalyst immobilized in polyacrylamide particles. The enzymatic hydration produces the desired amide at >99.3% selectivity at 100% conversion. While usage of the biocatalyst does provide a high conversion rate, it has been noted that these selectivites and conversions are ideally high for large industrial processes. However, for this process design, these conversions were used to model the best case scenario. Lower conversions of MPDA to niacinamide are investigated in the Sensitivity Analysis section later in the report.

Reactor Train 4 is designed as adiabatic, stirred-tank reactors using immobilized whole cells of R. rhodochrous *J1* employed in three stages. Sizing of the reactor was done via scaling up of the bench-scale data from the Lonza patent. It was determined that the three reactor tanks for Reactor 4 (R-202A, R-202B, and R-202C) will each have a carbon steel construction, an agitation rate of 110 rpm, a volume of 6,975 ft3, and will be operating at room temperature and pressure. The residence time of the whole cascade will be 12 hours, with 4 hours for each vessel (Nagasawa et al., 1988).

Mass of Biocatalyst

The dry weight of whole cell biocatalyst *R. rhodochrous* J1 immobilized in polyacrylamide particles was calculated via scaling up of the bench-scale data from the patent. It was determined that each 6,975 ft^3 tank would house 1,740 lb (dry weight) of the whole cell biocatalyst *R. rhodochrous* J1 immobilized in polyacrylamide particles. This is equivalent to 878.7 lb of immobilized enzyme, nitrile hydratase, NHase. The cell density of each reactor would then be 0.25 lb/ft^3. The total price of the catalyst is $153,910 for all three vessels. Refer to page 237 for Sample Calculations.

Cascade Choice

In terms of the cascade choice, Lonza investigated several process options including single-stage continuous fluidized bed, batch stirred tank, single-stage fed-batch stirred tank, single-stage continuous stirred tank, and multi-stage continuous stirred tank. Ultimately Lonza chose the multi-stage continuous stirred tank (Meyer & Ruesing, 2008). For this process, the reactor cascade will also be designed as such since Lonza has found that it optimizes the process.

Reactor Selection

Airlift reactors are unsuitable in this case because the airlift design could cause problems related to mixing and oxygen transfer especially when the polyacrylamide gels increase the weight and density of the biocatalysts. For this reason, the mechanically stirred tank design was used since it is usually preferred for larger-scale operations, has the advantage of operating at a low substrate level, and is suitable for substrate-inhibition reactions.

Agitator

The agitation rate in the reactors will be limited at 110 rpm to not disturb cell growth profiles and prevent cell membrane damage as high agitation rates can shear the cells. Furthermore, research has shown that specific product formation for bioprocesses is generally higher at lower impeller speeds (Doble, 2006). Two pitched blade turbines as agitators would be required for each vessel, each operating at 35 hp.

Process Modeling

Another set of simplifications occurred when dealing with the reaction vessels. Since specifications were not given on any of the first three reactors, they were modeled using the RSTOIC block in ASPEN. These reactors had the respective reactions added into them, assuming a certain conversion of the reaction. For the side reactions that may occur in the process, the third reactor, R-201, had a fraction of the 3-methylpyridine that is produced in that reactor essentially combust and form nitrogen, carbon dioxide, and water. This effectively accounts for the product lost in the process as well as the energy associated with these side products in the third reactor.

For the fourth reactor, R-202 (A,B, and C), RSTOIC was used to model the reaction that occurs within the three CSTR's in series. Due to constraints associated with ASPEN, it is difficult to correctly illustrate the actual design of this fourth reactor. For each of these reactors in the series, the vapor/liquid mixture from the previous step in the process is fed from the bottom through the CSTR to create a bubbling effect that ideally transfers the stream through the biocatalyst in the reactor. The same issue in modeling occurred at the outlet. No reactor in ASPEN can model a vapor and liquid stream exiting from the reactor. Therefore, a separation vessel was used as a dummy unit to model the reactor streams separating into two streams, a liquid and a vapor, when they exit each CSTR in the series. To keep these reaction vessels as close to 1 atm and 77°F, a pump moves the liquid fraction from the reactor while a blower is added to move the vapor stream. Heat exchangers were placed after the pump and blower before entering into the next reaction vessel.

Block (300): Niacinaide Purification

Summary

The third block in the process models the purification of niacin. After M-301 mixes the ammonia and water stream from A-102 earlier with the recycled stream of ammonia and water, the remainder of the organic molecules from the previous block mixes in as well. From the mixer, the stream goes to a heat exchanger where the temperature of the stream is brought down to close to room temperature. The stream enters the decolorizing unit, where the red dye leftover from the biocatalyst in the fourth reactor is removed with activated carbon. This stream then travels to the neutralizer where a mixture of ammonia and ammonium chloride create a buffer solution that effectively neutralizes the niacinamide formed in previous stages. Following this step, the stream is increased in pressure with a pump and then heated up to mix with the nitrogen streams coming in. Stream S-305 is heated nitrogen coming in to act as a drying agent in the dryer. This nitrogen stream is heated before continuing to the bottom of the dryer, effectively removing all the water and ammonia in the stream. The organic products, including the desired product niacinamide, fall out of the dryer as a solid product while the water, ammonia, and hot nitrogen leave the spray out of the top. This hot stream of ammonia, water, and nitrogen is compressed and then cooled to be separated in a flash vessel. From here, a portion of the nitrogen stream from the top of the flash vessel is purged while the remainder is fed back into the stream entering the dryer to help with the removal of water and ammonia in the streams. The water and ammonia mixture is also recycled back, whereas a portion of the stream is purged. The remaining mixture, S-318, is added into M-301 to be used again for the separation processes.

Specialized Equipment

Decolorizing Unit

R. rhodochrous J1 has a red pigment (DiCosimo, R., 2006). The decolorizing unit is required to remove the red pigment leftover from the biocatalyst in the fourth reactor. As such, the patent entitled *Method for purifying amide compounds by reacting with activated carbon under acidic conditions* is referred to when designing the column filled with activated carbon (Abe, T., et al., 2001). The unit is essentially an adsorption column, modeled as a vertical pressure vessel, and is filled with activated carbon. Correlations from *Product and Process Design Principles* were used to size and cost the entire unit—column and activated carbon. Knowing the volumetric flow rate to be 7.74 ft^3/min and assuming a 10 minute residence time in the column, the volume of material in the vessel is calculated to be 77 ft^3. Adjusting the volume for potential dissolved vapor, sufficient volume occupied by the catalyst, and increases in production capacity, the vessel volume is now 199 ft^3, and is thus sized as 4 ft in diameter and 16 ft in length. Void fraction of activated carbon is approximately 0.6. With this, the volume of activated carbon required is calculated and cost as shown in Sample Calculations page 239.

Dryer

Several different types of dryers were considered that would ultimately produce a final product that is of free-flowing powder, a form crucial for niacinamide packaging. The first type of dryer considered was a fluidized spray dryer. The continuous turbo-tray dryer (commercial Wyssmont TURBO-DRYER® system) was another such recommendation given by Mr. Fabiano. The Wyssmont TURBO-DRYER® can handle a range of materials including thick slurries continuously and is capable of providing a free-flowing product. Standard construction of the dryer can handle operating temperatures of up to 650°F, well above of our operating ranges. Furthermore, an advantage of the Wyssmont TURBO-DRYER® over fluidized spray drying equipment is that it can operate in a closed-circuit system. Size and costing was scaled-up using information obtained from examples of performance data given in Perry's and is presented in Table B1 below (Perry & Green, 2008).

Table B1. Wyssmont TURBO-DRYER® performance data

Material Dried	Niacinamide
Dried Product (lb/hr)	3372
Evaporation Rate (lb/hr)	650
Type of heating system	Steam
Heating medium	Hot gas
Drying medium	Inert gas
Materials of Construction	Stainless-steel interior
Dryer height (ft)	23
Dryer diameter (ft)	20
Recovery system	Shell-and-tube condenser
Condenser cooling medium	Chilled water
Location	Indoor
Purchase Cost	$ 804,369
Dryer assembly	Packaged unit

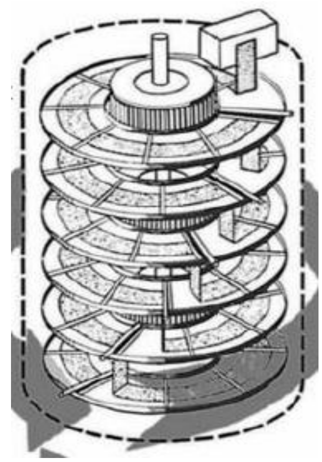


Figure 5. Wyssmont Turbo-Dryer; Source: Wyssmont Advertisement. Chemical Engineering, Access Intelligence. **May 2010**

Process Modeling

A decolorizer filled with activated carbon is needed for the third block of the process. However, ASPEN is unable to model a color change in the flowsheet, prompting the addition of a splitter with one of the streams equal to 0 fraction split. By doing this, the vessel could be sized and cost calculated given the ASPEN simulation results for the conditions into and out of the decolorizer. Directly after this vessel is a neutralizer, N-301. This RSTOIC models the reaction that takes the niacinamide that was produced earlier in the process and converts it, with water and ammonia, into the salt form of the niacin, ammonium nicotinate. A buffer solution consisting of NH_4Cl and NH_3 must be created in the vessel to properly neutralize the product. Because the only way to accurately calculate the components in the buffer solution, lab-scale analysis must be done while the process is running. Since the chloride present in the neutralizer would have little impact on the remainder of the process, it was left out of the ASPEN simulation. However, the neutralizer was modeled as an RSTOIC block to verify that the stoichiometric ratios of the reaction are already satisfied with the water and ammonia already created in the overall process. This made sure that the process would, under the right pH conditions, form the salt ammonium nicotinate, effectively neutralizing the solution.

Finally, the dryer was modeled in ASPEN as a SEP block unit. Since the dryer block in ASPEN was unable to work with this particular process design, a series of trial and error simulations were done to find the best unit within ASPEN to model the dryer. After the dryer specific model in ASPEN did not converge, a hierarchy block was added to convert the organic compounds previously defined as conventional components to solids. Then, when the dryer still did not converge, the same was done with a flash vessel. However, the separation in the flash vessel did not correctly model the dryer since most of these components turned into liquids rather than solids when the necessary temperatures were reached, around 387°F, whereas these components would be solids and fall out of the evaporated water and ammonia in actuality. For rough estimates of purity and solid niacin chemical composition, a SEP unit was finally decided to most accurately model the conditions and separation fractions of a dryer. All organics in the stream leave as stream S-316 while the water, ammonia, and nitrogen are evaporated to leave from the top of the vessel. The hot nitrogen mixture that enters through the bottom of the dryer evaporates water and ammonia leaving behind the remainder of the organics; this SEP unit, as compared to the rest of the models used in ASPEN, most closely resembles the lab-scale composition attained in patent references.

C. Equipment List and Unit Descriptions

Block (100)

Table C1. A list of equipment used in the process for Block (100).

Unit #	Equipment Type	Function	Operating T (°F)	Operating P (psia)
A-101	Absorber	Separates mainly H_2 and NH_3 from vapor stream (S-112) into S-113	C = 6 R = 366	40
A-102	Absorber	Separates mainly H2 from S-114 to S-115 via extraction with water in S-117	C = -118 R = 225	170
C-101	Compressor	Increases pressure of S-104 before running through R-101	560	ΔP=39 Discharge P = 73
C-102	Compressor	Increase pressure of distillate (S-107) of D-101 before feeding it to R-102	393	ΔP=58 Discharge P = 73
C-103	Compressor	Increase pressure of S-113 before running through A-102	314	ΔP=130 Discharge P = 170
D-101	Distillation Column	Separate MPDA from S-106 to be recycled	D = 266 B = 379	15
HX-101	Heat Exchanger	Increases temperature of S-103 for feed into R-101	527	34
HX-102	Heat Exchanger	Increases temperature of S-110 for feed into R-102	554	63
M-101	Mixer	Mixes streams S-102 and S-109 for feed into HX-101	81	44
P-101	Pump	Pumps S-101 to then run through HX-101 for MPDA vaporization	77	ΔP=29 Discharge P = 44
P-102	Pump	Pumps bottoms of D-101 (S-108) for MPDA recycle	380	ΔP=29 Discharge P = 44
P-103	Pump	Increases pressure of S-116 before running through A-102	91	ΔP=155 Discharge P = 170
R-101	Tubular Reactor	Converts MPDA to 3-methylpiperidine	581	72
R-102	Packed Bed Reactor	Converts 3-methylpiperidine to 3-picoline	554	42
T-101	Storage Tank	Stores the liquid MPDA as feed to the process	77	15
WS-102	Wet Scrubber	Removes NO_X and residual NH_3 out of the burning of S-115 so it can be vented to the atmosphere	210	48

Absorber (A-101)

A-101 is a 20-stage column for separating mainly the hydrogen and ammonia from vapor stream S-112 into S-113. The inlet stream enters at Stage 17. Temperature varies in the column from 266°F in the condenser (top stage) to 402°F in the reboiler (bottom stage).

The condenser is a partial-vapor fixed tube sheet heat exchanger that decreases the temperature of the overhead before sending it through a compressor (C-103). The hot stream on the shell side is cooled from 274°F (Stage 2) to 6°F (Stage 1/S-113). 6,411,900 lb/hr of refrigerant, R-134a, enters the tube side to cool the streams. The tube and shell side heat transfer coefficients are 250 and 2,632 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 226 ft^2. The total heat duty is -2.8 MMBtu/hr. There are 44 tubes of 20 ft. with an outer diameter of 1 in. The shell is 20 ft. in length and has a diameter of 10 in. with 16 baffles. With a carbon steel construction, the total bare-module cost of the condenser is $65,870.

The reboiler is a U-tube kettle vaporizer that uses high-pressure steam to vaporize a portion of the liquid bottoms product of the column. The distillate on the tube side is heated from 366°F (Stage 20) to 444°F. 1,401 lb/hr of steam at 450 psia enters the shell side to heat the cold streams. The tube and shell side heat transfer coefficients are 1,000 and 200 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 202 ft^2. The total heat duty is 1.7 MMBtu/hr. There are 39 tubes of 20 ft. with an outer diameter of 1 in. The shell is 13 ft. in length and has a diameter of 21 in. with 9 baffles. With a carbon steel construction, the total bare-module cost of the unit is $55,480.

With a carbon steel construction, the total bare-module cost of the entire unit is $3,291,000. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Absorber (A-101) specification sheet on page 66 and in Appendix IX on page 241.

Absorber (A-102)

A-102 is a 10-stage column for separating mainly hydrogen from S-114 to S-115 via extraction with water in S-117. The inlet stream S-114 enters at Stage 8 while the inlet stream S-117 enters at Stage 2. Temperature varies in the column from -118°F in the condenser (top stage) to 225°F in the reboiler (bottom stage). The column manages to remove all of the hydrogen and recovers >99% by mass of the ammonia in the inlet stream.

The condenser is a partial-vapor fixed tube sheet heat exchanger that decreases the temperature of the overhead before sending it through a compressor (C-103). It has a reflux ratio of 1. The hot stream on the shell side is cooled from 90°F (Stage 2) to -118°F (Stage 1/S-115). 2,799,830 lb/hr of refrigerant, ethylene, enters the tube side to cool the streams. The tube and shell side heat transfer coefficients are 250 and 1,019 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 177 ft^2. The total heat duty is -1.2 MMBtu/hr. There are 34 tubes of 20 ft. with an outer diameter of 1 in. The shell is 20 ft. in length and has a diameter of 10 in. with 16 baffles. With a carbon steel construction, the total bare-module cost of the condenser is $73,300.

The reboiler is a U-tube kettle vaporizer that uses high-pressure steam to vaporize a portion of the liquid bottoms product of the column. The distillate on the tube side is heated from 146°F (Stage 9) to 225°F (Stage 10). 682 lb/hr of steam at 450 psia enters the shell side to heat the streams. The tube and shell side heat transfer coefficients are 1,000 and 526 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 202 ft^2. The total heat duty is 0.8 MMBtu/hr. There are 6 tubes of 20 ft. with an outer diameter of 1 in. The shell is 13 ft. in length and has a diameter of 9 in. with 9 baffles. With a carbon steel construction, the total bare-module cost of the unit is $42,560.

With a carbon steel construction, the total bare-module cost of the entire unit is $2,284,000. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using

ASPEN Process Economic Analyzer (IPE). Please refer to the Absorber (A-102) specification sheet on page 67 and in Appendix IX on page 241.

Compressor (C-101)

C-101 is a rotary twin-screw compressor used to increase the pressure of the vapor stream S-104 by 39 psi, from 33.5 psia to 72.5 psia in S-105 before it is sent to the first reactor (R-101). The inlet volumetric flow rate is 144 ft^3/min. The power consumption of the unit is 25.3 HP. The compressor is powered using an electric motor drive that consumes 17 kW. With a cast-iron construction, the total bare-module cost of the unit is $86,720. Please refer to the Compressor (C-101) specification sheet on page 73 and the Sample Calculations in Appendix IX on page 248.

Compressor (C-102)

C-102 is a rotary twin-screw compressor used to increase the pressure of the vapor stream S-107 by 57.8 psi, from 14.7 psia to 72.5 psia in S-110 before it is sent to the heat exchanger (HX-102) to be heated. The inlet volumetric flow rate is 495 ft^3/min. The power consumption of the unit is 81.6 HP. The compressor is powered using an electric motor drive that consumes 55 kW. With a cast-iron construction, the total bare-module cost of the unit is $202,400. Please refer to the Compressor (C-102) specification sheet on page 74 and the Sample Calculations in Appendix IX on page 248.

Compressor (C-103)

C-103 is a rotary twin-screw compressor used to increase the pressure of the vapor stream S-113 by 130 psi, from 40 psia to 170 psia in S-114 before it is sent to absorber (A-102). The inlet volumetric flow rate is 235 ft^3/min. The power consumption of the unit is 111.5 HP. The compressor is powered using an electric motor drive that consumes 75 kW. With a cast-iron construction, the total bare-module cost of the unit is $253,750. Please refer to the Compressor (C-103) specification sheet on page 75 and the Sample Calculations in Appendix IX on page 248.

Distillation Column (D-101)

D-101 is a 40-stage column for separating out the leftover MPDA from S-106 to be recycled back through S-108. The inlet stream enters at Stage 33. Temperature varies in the column from 266°F in the condenser (top stage) to 402°F in the reboiler (bottom stage). The column recovers >99.9% by mass of the MPDA in the inlet stream. The number of stages required for the distillation column was obtained through ASPEN simulations. A purity for MPDA removal was specified and operating conditions for the column were optimized within ASPEN.

The condenser is a partial-vapor fixed tube sheet heat exchanger that decreases the temperature of the overhead before sending it through a compressor (C-102). The hot stream on the shell side is cooled from 306°F (Stage 2) to 266°F (Stage 1/S-107). 231,890 lb/hr of cooling water enters the tube side to cool the streams. The total heat duty is -6.9 MMBtu/hr. There are 52 tubes of 20 ft. with an outer diameter of 1 in. The shell is 20 ft. in length and has a diameter of 12 in. with 16 baffles. With a carbon steel construction, the total bare-module cost of the condenser is $59,060.

The reboiler is a U-tube kettle vaporizer that uses high-pressure steam to vaporize a portion of the liquid bottoms product of the distillation column. The distillate on the tube side is heated from 318°F (Stage 40) to 402°F (S-108). 5,368 lb/hr of steam at 450 psia enters the shell side to heat the streams. The tube and shell side heat transfer coefficients are 1,000 and 200 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 143 ft^2. The total heat duty is 6.4 MMBtu/hr. There are 176 tubes of 20 ft. with an outer diameter of 1 in. The shell is 13 ft. in length and has a diameter of 39 in. with 9 baffles. With a carbon steel construction, the total bare-module cost of the unit is $85,980.

With a carbon steel construction, the total bare-module cost of the entire unit is $4,023,800. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Distillation Column (D-101) specification sheet on page 77 in Appendix IX on page 241.

Heat Exchanger (HX-101)

HX-101 is a floating head shell-and-tube heat exchanger that models an evaporator that increases the temperature of the stream entering the first reactor R-101. S-103 on the tube side is heated from 81°F (S-103) to 527°F (S-104). 5,872 lb/hr of Dowtherm A enters the shell side to heat the streams. The tube and shell side heat transfer coefficients are 200 and 175 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 143 ft^2. The total heat duty is 1.5 MMBtu/hr. There are 27 tubes of 20 ft. with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 10 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $243,000. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-101) specification sheet on page 83 in Appendix IX on page 250.

Heat Exchanger (HX-102)

HX-102 is a floating head shell-and-tube heat exchanger that increases the temperature of the stream entering the second reactor R-102. S-110 on the tube side is heated from 393°F (S-110) to 554°F (S-111). 1,172 lb/hr of Dowtherm A enters the shell side to heat the streams. The tube and shell side heat transfer coefficients are 100 and 175 Btu/hr-ft2-°F respectively, leading to a total heat transfer area of 104 ft2. The total heat duty is 0.3 MMBtu/hr. There are 20 tubes of 20 ft. with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 8 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $236,800. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-102) specification sheet on page 84 in Appendix IX on page 250.

Pump (P-101)

P-101 is a centrifugal pump used to pump the liquid MPDA from storage tank T-101 through stream S-101 to S-102 to the mixer (M-101) and heat exchanger (HX-101) to be vaporized. For a pressure change of 29 psi, the head developed is 68 ft, and the net work required is 0.38 HP. With a carbon steel construction, the total bare-module cost of the unit is $100,806. Please refer to the Centrifugal Pump (P-101) specification sheet on page 98 and the Sample Calculations in Appendix IX on page 252.

Pump (P-102)

P-102 is a centrifugal pump used to pump the bottoms from distillation column D-101 through stream S-108 to S-109 to the mixer (M-101) to be recycled. For a pressure change of 23 psi, the head developed is 67 ft, and the net work required is 0.0038 HP. With a carbon steel construction, the total bare-module cost of the unit is $100,426. Please refer to the Centrifugal Pump (P-102) specification sheet on page 99 and the Sample Calculations in Appendix IX on page 252.

Pump (P-103)

P-103 is a centrifugal pump used to pump water through S-116 to the absorber (A-102) to absorb the ammonia incoming from S-114. For a pressure change of 155 psi, the head developed is 362 ft, and the net work required is 0.74 HP. With a carbon steel construction, the total bare-module cost of the unit is $138,090. Please refer to the Centrifugal Pump (P-103) specification sheet on page 100 and the Sample Calculations in Appendix IX on page 252.

Reactor 1 – Tubular Reactor (R-101)

In Reactor 1, the cyclization/deamination of MPDA to produce MPI with ammonia as a byproduct takes place at an overall conversion of 99 %. R-101 is comprised of four multitubular vessels with 15 tubes 685 ft in total length and nominal diameters of 6 inches, operating at 581°F and a pressure of 72.5 psia with a mass hourly space velocity (MHSV) of 0.6 lb/lb-hr over HZSM-5 catalysts. With a stainless steel shell-and-tube heat exchanger construction, the total heat transfer surface area is 17,800 ft^2. The total bare-module cost of the unit is $2,567,280. Please refer to the Reactor 1 (R-101) specification sheet on page 106.

Reactor 2 – Packed Bed Reactor (R-102)

In Reactor 2, the MPI produced in R-101 is converted to PIC at an overall conversion of 99% in an endothermic dehydrogenation reaction. Aforementioned this conversion is idealized; this conversion was only used because it is based on the experimental data given from the bench scale experiments for the process. R-102 is comprised of 40 tubes 20 ft in total length and nominal diameters of 4 inches, operating at 554°F and a pressure of 42 psia over 1% Pd-SiO2/Al2O3 catalysts. With a stainless steel shell-and-tube heat exchanger construction, the total heat transfer surface area is 838 ft2. The total bare-module cost of the unit is $97,360. Please refer to the Reactor 2 (R-102) specification sheet on page 107.

Feed Storage Tank (T-101)

T-101 is a floating roof storage tank that stores the liquid MPDA feed at ambient temperature and pressure. The tank has a storage capacity of 113,000 gallons of MPDA with a residence time of 7 days. MPDA is fed continuously from the tank to the system via S-101. The choice of the floating-roof tank is in compliance with current EPA regulations that dictate its usage for when, at the maximum atmospheric temperature at the plant site, the vapor pressure of the liquid is greater than 0.75 psia for storage of more than 40,000 gal. In our case, the vapor pressure is 2.5 psi at 275°F for 77,000 gallons. Using a cast-iron construction, the total bare-module cost of the unit is $629,610. Please refer to the Feed Storage Tank specification sheet on page 110 and the Sample Calculations in Appendix IX on page 254.

Block (200)

Table C2. A list of equipment used in the process for the 200 block.

Unit #	Equipment Type	Function	Operating T (°F)	Operating P (psi)
B-201	Blower	Increases pressure of S-208 before running through R-202B	251	ΔP=17 Discharge P = 32
B-202	Blower	Increases pressure of S-215 before running through R-202C	230	ΔP=15 Discharge P = 30
B-203	Blower	Increases pressure of S-220 before running through F-201	276	ΔP=22 Discharge P = 38
F-201	Flash Vessel	Initial separation of organic compounds from vapor products in S-227	32	15
HX-201	Heat Exchanger	Increases temperature of streams fed into R-201	626	30
HX-202A	Heat Exchanger	Decreases temperature of S-205 for feed into R-202A	100	19
HX-202B	Heat Exchanger	Decreases temperature of S-205 for feed into R-202A	77	19
HX-203	Heat Exchanger	Decreases temperature of S-212 before running through R-202B	77	20
HX-204	Heat Exchanger	Decreases temperature of S-219 before running through R-202C	77	20
HX-205	Heat Exchanger	Decreases temperature of S-226 before running through F-201	32	28
HX-206	Heat Exchanger	Increases temperature of S-230 before being fed into M-301	90	35
M-201	Mixer	Mixes streams S-119 and S-202 for subsequent feed into HX-201	79	30
M-202	Mixer	Mixes streams S-209 and S-211 for subsequent feed into HX-203	79	30
M-203	Mixer	Mixes streams S-216 and S-218 for subsequent feed into HX-204	79	38
M-204	Mixer	Mixes streams S-223 and S-225 for subsequent feed into HX-205	79	38
P-201	Pump	Increases pressure of S-210 before running through R-202B	77	ΔP=15 Discharge P = 30
P-202	Pump	Increases pressure of S-217 before running through R-202C	77	ΔP=15 Discharge P = 30
P-203	Pump	Increases pressure of S-224 before running through F-201	77	ΔP=30 Discharge P = 46

Unit #	Equipment Type	Function	Operating T (°F)	Operating P (psi)
P-204	Pump	Increases pressure of S-229 before running through HX-206	32	ΔP=30 Discharge P = 45
R-201	Tubular Reactor	Converts 3-picoline to 3-cyanopyridine and water	626	29
R-202A	Semi-continuous stirred tank reactor	Converts 3-cyanopyridine to niacinamide (niacin)	77	15
R-202B	Semi-continuous stirred tank reactor	Converts 3-cyanopyridine to niacinamide (niacin)	77	15
R-202C	Semi-continuous stirred tank reactor	Converts 3-cyanopyridine to niacinamide (niacin)	77	16
SP-201	Splitter	Models the control valves used to split the flow of S-118	225	170

Blower (B-201)

B-201 is a centrifugal blower used to increase the pressure of the vapor stream S-208 by 17.3 psi, from 14.6 psia to 31.9 psia in S-209 before it is sent to the heat exchanger HX-203 to be slightly cooled. The power consumption of the unit is 2.8 HP. With a cast-iron construction, the total bare-module cost of the unit is $5,490. Please refer to the Blower (B-201) specification sheet on page 70 and the Sample Calculations in Appendix IX on page 247.

Blower (B-202)

B-202 is a centrifugal blower used to increase the pressure of the vapor stream S-215 by 15 psi, from 15.1 psia to 30.1 psia in S-216 before it is sent to the heat exchanger HX-204 to be slightly cooled. The power consumption of the unit is 2.5 HP. With a cast-iron construction, the total bare-module cost of the unit is $4,950. Please refer to the Blower (B-202) specification sheet on page 71 and the Sample Calculations in Appendix IX on page 247.

Blower (B-203)

B-203 is a centrifugal blower used to increase the pressure of the vapor stream S-222 by 22 psi, from 15.6 psia to 37.6 psia in S-223 before it is sent to the heat exchanger HX-205 to be slightly cooled. The power consumption of the unit is 3.2 HP. With a cast-iron construction, the total bare-module cost of the unit is

$6,080. Please refer to the Blower (B-203) specification sheet on page 72 and the Sample Calculations in Appendix IX on page 247.

Flash Vessel (F-201)

F-201 is a vertical flash vessel for the separation of organic compounds from vapor products (mainly O_2) in S-227. The unit operates at 32°F and 15 psia with a residence time of 5 minutes. The height and diameter of the vessel is 12 and 3 ft respectively. With a steel (ASTM A516) construction, the total bare-module cost of the unit is $535,640. Please refer to the Flash Vessel (F-201) specification sheet on page 81 and the Sample Calculations in Appendix IX on page 249.

Heat Exchanger (HX-201)

HX-201 is a floating head shell-and-tube heat exchanger that increases the temperature of the stream entering the third reactor R-201. S-203 on the tube side is heated from 159°F (S-203A) to 626°F (S-203). 10,400 lb/hr of Dowtherm A enters the shell side to heat the streams. The tube and shell side heat transfer coefficients are 200 and 143 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 209 ft^2. The total heat duty is 2.6 MMBtu/hr. There are 40 tubes of 20 ft. with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 10 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $424,600. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-201) specification sheet on page 85 in Appendix IX on page 250.

Heat Exchanger (HX-202A)

HX-202A is a floating head shell-and-tube heat exchanger that models a partial condenser that decreases the temperature of the stream entering the first vessel of reaction train 4 (R-202A). The hot stream on the shell side is cooled from 626°F (S-205) to 100°F (S-206A). 146,390 lb/hr of cooling water enters the tube side to cool the streams. The tube and shell side heat transfer coefficients are 1,050 and 1,020 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 146 ft^2. The total heat duty is -4.4 MMBtu/hr.

There are 28 tubes of 20 ft. with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 10 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $330,700. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-202A) specification sheet on page 86 in Appendix IX on page 250.

Heat Exchanger (HX-202B)

HX-202B is a floating head shell-and-tube heat exchanger that again models a partial condenser that further decreases the temperature of the stream entering the first vessel of reaction train 4 (R-202A). The hot stream on the shell side is cooled from 100°F (S-206A) to 77°F (S-206). 2,170,000 lb/hr of refrigerant enters the tube side to cool the streams. The tube and shell side heat transfer coefficients are 1,050 and 470 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 224 ft^2. The total heat duty is -95,180 Btu/hr. There are 43 tubes of 20 ft. with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 12 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $244,500. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-202B) specification sheet on page 87 in Appendix IX on page 250.

Heat Exchanger (HX-203)

HX-203 is a floating head shell-and-tube heat exchanger that models a partial condenser which decreases the temperature of the stream entering the second vessel of reactor train 4 (R-202B). The hot stream on the shell side is cooled from 79°F (S-212) to 77°F (S-213). 16,580 lb/hr of refrigerant enters the tube side to cool the streams. The tube and shell side heat transfer coefficients are 250 and 303 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 5 ft^2. The total heat duty is -7,220 Btu/hr. There is one 20 ft. tube with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 3 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $182,700. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using

ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-203) specification sheet on page 88 in Appendix IX on page 250.

Heat Exchanger (HX-204)

HX-204 is a floating head shell-and-tube heat exchanger that decreases the temperature of the stream, acting as a partial condenser, entering the third vessel of reactor train 4 (R-202C). The hot stream on the shell side is cooled from 79°F (S-219) to 77°F (S-220). 14,830 lb/hr of refrigerant enters the tube side to cool the streams. The tube and shell side heat transfer coefficients are 250 and 303 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 5 ft^2. The total heat duty is -6,460 Btu/hr. There is one 20 ft. tube with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 3 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $182,700. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-204) specification sheet on page 89 in Appendix IX on page 250.

Heat Exchanger (HX-205)

HX-205 is a floating head shell-and-tube heat exchanger that models a partial condenser that decreases the temperature of the stream entering the vapor liquid separator (F-201). The hot stream on the shell side is cooled from 79°F (S-226) to 32°F (S-227). 422,000 lb/hr of refrigerant enters the tube side to cool the streams. The tube and shell side heat transfer coefficients are 250 and 470 Btu/hr-ft2-°F respectively, leading to a total heat transfer area of 28 ft2. The total heat duty is -185,800 Btu/hr. There are five 20 ft. tubes with outer diameters of 1 in. The shell is 22 ft. in length and has a diameter of 6 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $230,200. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-205) specification sheet on page 90 in Appendix IX on page 250.

Heat Exchanger (HX-206)

HX-206 is a floating head shell-and-tube heat exchanger that increases the temperature of the bottoms leaving the vapor liquid separator (F-201). S-230 on the tube side is heated from 32°F (S-230) to 90°F (S-231). 185 lb/hr of hot water at 100°F enters the shell side to heat the streams. The tube and shell side heat transfer coefficients are 1,000 and 303 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 6 ft^2. The total heat duty is 223,490 Btu/hr. There is one 20 ft. tube with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 3 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $169,200. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-206) specification sheet on page 91 in Appendix IX on page 250.

Pump (P-201)

P-201 is a centrifugal pump used to pump liquid stream S-210 to be mixed, cooled, and sent to the second reactor in the cascade of reaction train 4. For a pressure change of 15 psi, the head developed is 29 ft, and the net work required is 0.28 hp. With a carbon steel construction, the total bare-module cost of the unit is $113,740. Please refer to the Centrifugal Pump (P-201) specification sheet on page 101 and the Sample Calculations in Appendix IX on page 252.

Pump (P-202)

P-202 is a centrifugal pump used to pump liquid stream S-217 to be mixed, cooled, and sent to the third reactor in the cascade of reaction train 4. For a pressure change of 15 psi, the head developed is 29 ft, and the net work required is 0.28 hp. With a carbon steel construction, the total bare-module cost of the unit is $113,740. This pump has the same specifications as P-201. Therefore, two of the same pumps can be purchased for P-201 and P-202. Please refer to the Centrifugal Pump (P-202) specification sheet on page 102 and the Sample Calculations in Appendix IX on page 252.

Pump (P-203)

P-203 is a centrifugal pump used to pump liquid stream S-224 to be mixed, cooled, and sent to the vapor liquid separator (F-201). For a pressure change of 30 psi, the head developed is 58 ft, and the net work required is 0.56 hp. With a carbon steel construction, the total bare-module cost of the unit is $113,740. Please refer to the Centrifugal Pump (P-203) specification sheet on page 103 and the Sample Calculations in Appendix IX on page 252.

Pump (P-204)

P-204 is a centrifugal pump used to pump liquid stream S-229 to be heated through by the heat exchanger (HX-206). For a pressure change of 30 psi, the head developed is 57 ft, and the net work required is 0.55 hp. With a carbon steel construction, the total bare-module cost of the unit is $103,090. This pump has the same specifications as P-203. Therefore, two of the same pumps can be purchased for P-203 and P-204. Please refer to the Centrifugal Pump (P-204) specification sheet on page 104 and the Sample Calculations in Appendix IX on page 252.

Reactor 3 (R-201)

In the third reactor, the exothermic ammoxidation to produce 3-cyanopyridines (and water as a byproduct) using ammonia and oxygen with PIC takes place at an overall conversion of 99%. As mentioned before, the high conversion rates are taken as an ideal case for the design process. These conversion rates were seen in the bench-scale experiments for the Lonza patent process. R-201 is comprised of 2,000 tubes 42 ft in total length and diameters of 1.8 inches, operating at 554°F and a pressure of 42 psia over V_2O_5, TiO_2, ZrO_2, and MoO_3 catalysts. With a stainless steel shell-and-tube heat exchanger construction, the total heat transfer surface area is 39,580 ft^2. The total bare-module cost of the unit is $2,286,270. Please refer to the Reactor 3 (R-201) specification sheet on page 108.

Reactor 4 (R-202A,B,C)

In Reactor 4, the biohydrolysis of 3-cyanopyridine produces niacinamide and water as a byproduct with an overall conversion of 99%. R-202A is the first in a series of three stirred-tank semi-batch reactors with a continuous feed of 3-cyanopyridine via S-206 at concentrations of between 10–20 wt% in the direction of process flow. The reactor also houses the whole cell biocatalyst *R. rhodochrous* J1 immobilized in polyacrylamide particles. The enzymatic hydration produces the desired amide at >99.3% selectivity at 100% conversion. The reactors have a volume of 6,975 ft^3 each and a residence time of 4 hours each, and will operate at 77°F and 15 psia. Each vessel will be equipped with two turbine agitators with an agitation rate of 110 rpm for each impeller. With a carbon steel (SA-285 Grade C) construction, the total bare-module cost of one unit is $918,160 making the total bare-module cost of the entire cascade to be $2,754,480. Please refer to the Stirred Tank Reactor specification sheet on page 109 and the Sample Calculations in Appendix IX on page 253.

Block (300)

Table C3. A list of equipment used in the process for the 300 block.

Unit #	Equipment Type	Function	Operating T (°F)	Operating P (psi)
AS-301	Packed Bed Air Stripper	Removes NH3 from S-319 so that the excess water can be release to surroundings	68	15
C-301	Compressor	Increases pressure of S-310 before entering HX-304	887	ΔP=54 Discharge P=68
DC-301	Decolorizing Unit	Removed red dye leftover from biocatalyst in R-202	77	20
DR-301	Dryer	Allows heated nitrogen to separate the mixture in S-307 to product in S-316 and recycled S-310	387	15
F-301	Flash Vessel	Separate N2 for recycle to the dryer; remainder to stream to liquid recycle, feed is S-312	32	58
HX-301	Heat Exchanger	Increases temperature of S-301 before running through DC-301	77	25
HX-302	Heat Exchanger	Increases temperature of S-306 before running through DR-301	392	30
HX-303	Heat Exchanger	Increases temperature of S-308 before running through DR-301	392	20
HX-304A	Heat Exchanger	Decreases temperature of S-311 before entering F-301	100	63
HX-304B	Heat Exchanger	Decreases temperature of S-311 before entering F-302	32	58
M-301	Mixer	Mixes the streams entering (S-201, S-231, S-318)	31	35
P-301	Pump	Increases pressure of S-305 before running through HX-302	77	ΔP=25 Discharge P=40
SP-301	Splitter	Models the control valves used to split S-317 into a purge and recycled stream	32	48
SP-302	Splitter	Models the control valves used to split S-313 into a purge and recycled stream	32	48
T-301	Storage Tank	Stores the free-flowing powder form of the niacinamide product exiting S-316	77	15
WS-301	Wet Scrubber	Cleans ammonia out of S-314 so it can be vented to the atmosphere	210	48

Compressor (C-301)

C-301 is a centrifugal compressor used to increase the pressure of the vapor stream S-310 by 53.5 psi, from 14.5 psia to 68 psia in S-311 before it is sent to the heat exchanger (HX-304A). The inlet volumetric flow rate is 12,915 ft^3/min. The power consumption of the unit is 2,253 HP. With a cast-iron construction, the total bare-module cost of the unit is $2,331,340. Please refer to the Compressor (C-301) specification sheet on page 76 and the Sample Calculations in Appendix IX on page 248.

Decolorizing Unit (DC-301)

DC-301 is a vertical vessel filled with activated carbon that acts as an adsorption column to remove the red pigment found in S-302. The unit operates at 77°F and 25 psia. The unit was modeled as a vertical pressure vessel. The height and diameter of the vessel is 16 and 4 ft respectively. With a carbon steel (SA-285 Grade C) construction, the total bare-module cost of the unit is $149,787. Please refer to the Decolorizing Unit (DC-301) specification sheet on page 79 and the Sample Calculations in Appendix IX on page 239 and page 251.

Dryer (DR-301)

DR-301 is a commercial Wyssmont TURBO-DRYER® system that dries the wet stream of niacinamide (S-307) to its final form of free-flowing powder (S-316). The drying medium used is a hot inert stream of nitrogen gas from S-309. The system has an evaporation rate of 650 lb/hr. With a stainless steel interior, the total bare-module cost of the unit is $1,657,000. Please refer to the Dryer specification sheet on page 80.

Flash Vessel (F-301)

F-301 is a vertical flash vessel to separate the nitrogen to be recycled back via S-313 and ammonia and water to be recycled back via S-317. The unit operates at 32°F and 58 psia with a residence time of 5 minutes. The height and diameter of the vessel is 12 and 4 ft respectively. With a steel (ASTM A516) construction, the total bare-module cost of the unit is $479,540. Please refer to the Flash Vessel (F-301) specification sheet on page 82 and the Sample Calculations in Appendix IX on page 249.

Heat Exchanger (HX-301)

HX-301 is a floating head shell-and-tube heat exchanger that increases the temperature of stream S-302 entering the decolorizing unit (DC-301). S-301 on the tube side is heated from 31°F (S-301) to 77°F (S-302). 1,020 lb/hr of hot water at 100°F enters the shell side to heat the streams. The tube and shell side heat transfer coefficients are 1,000 and 1,050 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 21 ft^2. The total heat duty is 1.24 MMBtu/hr. There are four 20 ft. tubes with outer diameters of 1 in. The shell is 22 ft. in length and has a diameter of 4 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $210,100. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-301) specification sheet on page 92 in Appendix IX on page 250.

Heat Exchanger (HX-302)

HX-302 is a floating head shell-and-tube heat exchanger that models an evaporator which increases the temperature of stream S-307 entering the dryer (DR-301). S-306 on the tube side is heated from 77°F (S-306) to 392°F (S-307). 24,000 lb/hr of steam at 450 psia enters the shell side to heat the streams. The tube and shell side heat transfer coefficients are 1,000 and 530 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 950 ft^2. The total heat duty is 28.9 MMBtu/hr. There are 182 tubes of 20 ft. in length with outer diameters of 1 in. The shell is 22 ft. in length and has a diameter of 20 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $391,400. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-302) specification sheet on page 93 in Appendix IX on page 250.

Heat Exchanger (HX-303)

HX-303 is a floating head shell-and-tube heat exchanger that increases the temperature of stream S-309 entering the dryer (DR-301). S-308 on the tube side is heated from 77°F (S-308) to 392°F (S-309). 2 lb/hr of steam at 450 psia enters the shell side to heat the streams. The tube and shell side heat transfer coefficients are 1,000 and 30 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 5 ft^2. The total heat duty is 2,430 Btu/hr. There is one 20 ft. tube with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 3 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $180,100. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-303) specification sheet on page 94 in Appendix IX on page 250.

Heat Exchanger (HX-304A)

HX-304A is a floating head shell-and-tube heat exchanger, modeling a partial condenser, decreases the temperature of the stream leaving the dryer (DR-301). The hot stream on the shell side is cooled from 887°F (S-311) to 100°F (S-312A). S-311 is at an unusually high temperature because the compressor preceding this heat exchanger increases the temperature of the stream from 387°F to 887°F with the pressure increase of 53.5 psi. 1,099,000 lb/hr of cooling water enters the tube side to cool the streams. The tube and shell side heat transfer coefficients are 1050 and 265 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 1411 ft^2. The total heat duty is -32.8 MMBtu/hr. There are 270 tubes of 20 ft. with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 24 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $802,500. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-304A) specification sheet on page 95 in Appendix IX on page 250.

Heat Exchanger (HX-304B)

HX-304B is a floating head shell-and-tube heat exchanger that also acts as a partial condenser which further decreases the temperature of the stream leaving the dryer (DR-301) before it enters the vapor liquid separator (F-301). The hot stream on the shell side is cooled from 100°F (S-312A) to 32°F (S-312). 3,997,250 lb/hr of refrigerant enters the tube side to cool the streams. The tube and shell side heat transfer coefficients are 250 and 470 Btu/hr-ft^2-°F respectively, leading to a total heat transfer area of 242 ft^2. The total heat duty is -1.75 MMBtu/hr. There are 47 tubes of 20 ft. with an outer diameter of 1 in. The shell is 22 ft. in length and has a diameter of 12 in. with 18 baffles. With a carbon steel construction, the total bare-module cost of the unit is $280,300. All calculations were performed using ASPEN Plus Exchanger Design and Rating (EDR) and cost using ASPEN Process Economic Analyzer (IPE). Please refer to the Heat Exchanger (HX-304B) specification sheet on page 96 and in Appendix IX on page 250.

Neutralizer (N-301)

N-301 is a vertical vessel that neutralizes the product stream, forming a slurry of ammonium nicotinate that dissolves in ammonia. The unit operates at 77°F and 20 psia. The unit was modeled as a vertical pressure vessel with agitators. The height and diameter of the vessel is 14.2 and 3.5 ft respectively. The vessel is fitted with two pitched blade turbines, each requiring a power of 2.89 hp, rotating at 200 rpm to mix the contents of the vessel well, ensuring thorough solubility. With a carbon steel (SA-285 Grade C) construction, the total bare-module cost of the unit is $142,700. Please refer to the Neutralizer (N-301) specification sheet on page 97 and the Sample Calculations in Appendix IX on page 251 and page 245.

Centrifugal Pump (P-301)

P-301 is a centrifugal pump used to pump liquid stream S-305 from the neutralizer to be heated through by the heat exchanger (HX-302) before being sent to the dryer. For a pressure change of 25 psi, the head developed is 56 ft, and the net work required is 1.7 hp. With a carbon steel construction, the total bare-module cost of the unit is $120,600. Please refer to the Centrifugal Pump (P-301) specification sheet on page 105 and the Sample Calculations in Appendix IX on page 252.

Product Storage Bin (T-301)

T-301 is a cone roof storage bin for the free-flowing powder form of the niacinamide product at ambient temperature and pressure. The bin has a storage capacity of 93,000 gallons of niacinamide with a residence time of 7 days. Niacinamide enters the bin continuously via S-316. Using a carbon steel construction, the total bare-module cost of the unit is $434,000. Please refer to the Product Storage Tank specification sheet on page 111 and the Sample Calculations in Appendix IX on page 254.

Mixers (M-101, M-201, M-202, M-203, M-204, M-301) and Splitters (SP-201, SP-301, SP-302)

All the mixers and splitters in the process are T's in the pipeline. No purchase cost is associated with the splitters and mixers as they are merely pipeline.

Mixers are used to mix multiple streams together before they are fed into unit equipment:

M-101 mixes S-102 and S-109 for feed into HX-101;

M-201 mixes streams S-119 and S-202 for subsequent feed into HX-201;

M-202 mixes streams S-209 and S-211 for subsequent feed into HX-203;

M-203 mixes streams S-216 and S-218 for subsequent feed into HX-204;

M-204 mixes streams S-223 and S-225 for subsequent feed into HX-205;

M-301 combines split stream S-201, S-231, and recycle stream S-318 to be fed into HX-301.

Splitters are used to redirect part of a well flow fluid circulation from its regular practice to smaller pipelines by managing a sequence of control valves:

SP-201 splits S-118 into two streams (S-201, fraction of 0.011, and S-202, fraction of 0.989) in which S-202 contains the excess flow of reactants not needed in the reaction;

SP-301 splits S-317 to a purge (S-319, fraction of 0.1) and recycle stream (S-318, fraction of 0.9);

SP-302 splits S-313 to a purge (S-314, fraction of 0.1) and recycle stream (S-315, fraction of 0.9).

D. EQUIPMENT SPECIFICATION SHEETS

The following pages list the specification sheets that detail each unit in the process.

Table D1. Equipment specifications table of contents

Absorber					
Identification:	Item:	*Absorber*			
	Item No.:	*A-101*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*791,116**		C_{BM} ($):	*3,291,044*
Function: Separates O_2, H_2 and N_2 from ammonia, water, niacinamide and the remaining heavy components in the bottoms.					
Operation: Continuous					

	S-112 Inlet	*Bottoms S-119 Outlet*	*Overhead S-113 Outlet*		
Materials Handled:					
Total Flow (lb/hr):	3,307	2,650	656		
Volumetric Flow (ft^3/hr):	36,436	54	14,104		
Component Flows (lb/hr):					
O_2	0	0	0		
H_2	170	Trace	170		
N_2	0	0	0		
Ammonia	485	Trace	485		
H_2O	0	0	0		
CO_2	0	0	0		
MPDA	0.002	0.002	Trace		
3-methylpiperidine	28	0.07	28		
3-picoline	2,624	2,624	1		
3-cyanopyridine	0	0	0		
Niacinamide	0	0	0		
Temperature (°F):	554	366	6		
Pressure (psi):	42.2	40	40		
Vapor Fraction:	1	<0.001	1		

Design Data:

Type:	Absorption Column
Material:	Carbon Steel
Length (ft):	20.0
Diameter (in):	10.0
Number of stages:	20

Utilities:

450 psi Steam (lb/hr):	1,401
Refrigeration (ton/day):	76,943

Comments: * cost reflects emtire unit incl. condenser and reboiler

Condenser

Identification:	Item:	*Fixed Tube Sheet Heat Exchanger*			
	Item No.:	*A-101-condenser*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
				C_{BM} ($):	*65,870*

Design Data:

Type:	Heat Exchanger		Tube	
Refux Ratio:	1		Number of tubes:	44
$T_{h,i}$ (°F):	274	Stage 2	Length (ft):	20
$T_{h,o}$ (°F):	6	Stage 1 / S-113	D_o (in):	1
Tube side h (Btu/hr-ft^2):	250		Shell	
Shell side h (Btu/hr-ft^2):	2632		Length (ft):	20
Total heat transfer A (ft^2):	226		D (in):	10
Total heat duty (MMBtu/hr):	-2.8		Number of baffles:	16
Material:	Carbon Steel			

Reboiler

Identification:	Item:	*U-tube kettle vaporizer*			
	Item No.:	*A-101-reboiler*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
				C_{BM} ($):	*55,480*

Design Data:

Type:	Heat Exchanger		Tube	
			Number of tubes:	39
$T_{c,i}$ (°F):	366	Stage 20	Length (ft):	20
$T_{c,o}$ (°F):	444		D_o (in):	1
Tube side h (Btu/hr-ft^2):	1000		Shell	
Shell side h (Btu/hr-ft^2):	200		Length (ft):	13
Total heat transfer A (ft^2):	202		D (in):	21
Total heat duty (MMBtu/hr):	1.7		Number of baffles:	9
Material:	Carbon Steel			

Absorber					
Identification:	Item:	*Absorber*			
	Item No.:	*A-102*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*548,989*		C_{BM} ($):	*2,283,795*
Function: Separates H_2 via extraction with water					
Operation: Continuous					

	Inlet (S-114)	*Inlet (S-117)*	*Outlet (S-118)*	*Outlet (S-115)*
Materials Handled:				
Total Flow (lb/hr):	656	1,200	1682	175
Volumetric Flow (ft^3/hr):	5,536	19	35	1845
Component Flows (lb/hr):				
O_2	0	0	0	0
H_2	170	0	Trace	170
N_2	0	0	0	0
Ammonia	485	0	481	4
H_2O	0	1200	1200	Trace
CO_2	0	0	0	0
MPDA	Trace	0	0	0
3-methylpiperidine	Trace	0	Trace	Trace
3-picoline	1	0	1	Trace
3-cyanopyridine	0	0	0	0
Niacinamide	0	0	0	0
Temperature (°F):	314	91	225	-118
Pressure (psi):	170	170	170	170
Vapor Fraction:	1	0	<0.001	1

Design Data:

Type:	Absorption Column
Material:	Carbon Steel
Length (ft):	20.0
Diameter (in):	10.0
Number of stages:	10

Utilities:

450 psi Steam (lb/hr):	682
Refrigeration (ton/day):	33,598

Comments: * cost reflects emtire unit incl. condenser and reboiler

Condenser							
Identification:	Item:	*Fixed Tube Sheet Heat Exchanger*					
	Item No.:	*A-102-condenser*				Date:	*4/10/13*
	No. Required:	*1*				By:	*JS/AC/PB/AL*
						C_{BM} ($):	*73,300*
Design Data:							
Type:	Heat Exchanger			Tube			
Refux Ratio:	1			Number of tubes:	34		
$T_{h,i}$ (°F):	90	Stage 2		Length (ft):	20		
$T_{h,o}$ (°F):	-118	Stage 1 / S-113		D_o (in):	1		
Tube side h (Btu/hr-ft^2):	250			Shell			
Shell side h (Btu/hr-ft^2):	1019			Length (ft):	20		
Total heat transfer A (ft^2):	177			D (in):	10		
Total heat duty (MMBtu/hr):	-1.2			Number of baffles:	16		
Material:	Carbon Steel						

Reboiler							
Identification:	Item:	*U-tube kettle vaporizer*					
	Item No.:	*A-102-reboiler*				Date:	*4/10/13*
	No. Required:	*1*				By:	*JS/AC/PB/AL*
						C_{BM} ($):	*42,560*
Design Data:							
Type:	Heat Exchanger			Tube			
				Number of tubes:	6		
$T_{c,i}$ (°F):	146	Stage 9		Length (ft):	20		
$T_{c,o}$ (°F):	225	Stage 10		D_o (in):	1		
Tube side h (Btu/hr-ft^2):	1000			Shell			
Shell side h (Btu/hr-ft^2):	526			Length (ft):	13		
Total heat transfer A (ft^2):	202			D (in):	9		
Total heat duty (MMBtu/hr):	0.8			Number of baffles:	9		
Material:	Carbon Steel						

Centrifugal Blower

Identification:	Item:	*Blower*			
	Item No.:	*B-201*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*2,555*		C_{BM} ($):	*5,492*

Function: Maintains pressure for stream S-208.

Operation: Continuous

	S-208 *Inlet*	*S-209* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	148	148			
Volumetric Flow (ft^3/hr):	1,802	1,096			
Component Flows (lb/hr):					
O_2	135	135			
H_2	0	0			
N_2	0.4	0.4			
Ammonia	0.004	0.004			
H_2O	3	3			
CO_2	7	7			
MPDA	Trace	Trace			
3-methylpiperidine	2	2			
3-picoline	0.7	0.7			
3-cyanopyridine	0.1	0.1			
Niacinamide	Trace	Trace			
Temperature (°F):	77	251			
Pressure (psi):	14.6	31.9			
Vapor Fraction:	1	1			

Design Data:

Material:	Cast Iron
Net Work Requirement (hp):	2.8
ΔPressure (psi):	17.3
Compression Ratio:	2.2

Utilities:

Electricity (kW):	1.7

Comments:

Centrifugal Blower

Identification:	Item:	*Blower*		
	Item No.:	*B-202*	Date:	*4/10/13*
	No. Required:	*1*	By:	*JS/AC/PB/AL*
	C_p ($):	*2,304*	C_{BM} ($):	*4,954*

Function: Maintains pressure for stream S-215.

Operation: Continuous

	S-215 *Inlet*	*S-216* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	148	148			
Volumetric Flow (ft^3/hr):	1,740	1,123			
Component Flows (lb/hr):					
O_2	135	135			
H_2	0	0			
N_2	0.4	0.4			
Ammonia	0.004	0.004			
H_2O	3	3			
CO_2	7	7			
MPDA	Trace	Trace			
3-methylpiperidine	2	2			
3-picoline	0.7	0.7			
3-cyanopyridine	0.1	0.1			
Niacinamide	Trace	Trace			
Temperature (°F):	77	230			
Pressure (psi):	15.1	30.1			
Vapor Fraction:	1	1			

Design Data:

Material:	Cast Iron
Net Work Requirement (hp):	2.5
ΔPressure (psi):	15
Compression Ratio:	2.0

Utilities:

Electricity (kW):	1.5

Comments:

Centrifugal Blower

Identification:	Item:	*Blower*		
	Item No.:	*B-203*	Date:	*4/10/13*
	No. Required:	*1*	By:	*JS/AC/PB/AL*
	C_p ($):	*2,828*	C_{BM} ($):	*6,080*

Function: Maintains pressure for stream S-208.

Operation: Continuous

	S-222 *Inlet*	*S-223* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	148	148			
Volumetric Flow (ft^3/hr):	1,682	959			
Component Flows (lb/hr):					
O_2	135	135			
H_2	0	0			
N_2	0.4	0.4			
Ammonia	0.004	0.004			
H_2O	3	3			
CO_2	7	7			
MPDA	Trace	Trace			
3-methylpiperidine	2	2			
3-picoline	0.7	0.7			
3-cyanopyridine	0.1	0.1			
Niacinamide	Trace	Trace			
Temperature (°F):	77	276			
Pressure (psi):	15.6	37.6			
Vapor Fraction:	1	1			

Design Data:

Material:	Cast Iron
Net Work Requirement (hp):	3.2
ΔPressure (psi):	22
Compression Ratio:	2.4

Utilities:

Electricity (kW):	2.0

Comments:

Centrifugal Compressor

Identification:	Item:	*Compressor*			
	Item No.:	*C-101*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*40,335*		C_{BM} ($):	*86,719*

Function: Maintains pressure for stream S-104.

Operation: Continuous

	S-104 *Inlet*	*S-105* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	3,340	3,340			
Volumetric Flow (ft^3/hr):	8,642	3,915			
Component Flows (lb/hr):					
O_2	0	0			
H_2	0	0			
N_2	0	0			
Ammonia	Trace	Trace			
H_2O	0	0			
CO_2	0	0			
MPDA	3,340	3,340			
3-methylpiperidine	0.002	0.002			
3-picoline	0	0			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	527	560			
Pressure (psi):	33.5	72.5			
Vapor Fraction:	1	1			

Design Data:

Material:	Cast Iron
Net Work Requirement (hp):	25.3
ΔPressure (psi):	39
Compression Ratio:	2.2

Utilities:

Electricity (kW):	16.5

Comments:

Centrifugal Compressor						
Identification:	Item:	*Compressor*				
	Item No.:	*C-102*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*94,138*			C_{BM} ($):	*202,397*
Function: Maintains pressure for stream S-104.						
Operation: Continuous						
	S-107 *Inlet*	*S-110* *Outlet*				
Materials Handled:						
Total Flow (lb/hr):	3,307	3,307				
Volumetric Flow (ft^3/hr):	30,087	7,563				
Component Flows (lb/hr):						
O_2	0	0				
H_2	0	0				
N_2	0	0				
Ammonia	485	485				
H_2O	0	0				
CO_2	0	0				
MPDA	0.002	0.002				
3-methylpiperidine	2,822	2,822				
3-picoline	0	0				
3-cyanopyridine	0	0				
Niacinamide	0	0				
Temperature (°F):	266	393				
Pressure (psi):	14.7	72.5				
Vapor Fraction:	1	1				
Design Data:						
Material:	Cast Iron					
Net Work Requirement (hp):	81.6					
ΔPressure (psi):	17.3					
Compression Ratio:	4.9					
Utilities:						
Electricity (kW):	54.6					
Comments:						

Centrifugal Compressor

Identification:

Item:	*Compressor*		
Item No.:	*C-103*	Date:	*4/10/13*
No. Required:	*1*	By:	*JS/AC/PB/AL*
C_p ($):	*118,025*	C_{BM} ($):	*253,753*

Function: Maintains pressure for stream S-113.

Operation: Continuous

	S-113 *Inlet*	*S-114* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	656	656			
Volumetric Flow (ft^3/hr):	14,104	5,536			
Component Flows (lb/hr):					
O_2	0	0			
H_2	170	170			
N_2	0	0			
Ammonia	485	485			
H_2O	0	0			
CO_2	0	0			
MPDA	Trace	Trace			
3-methylpiperidine	Trace	Trace			
3-picoline	1	1			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	6	314			
Pressure (psi):	40	170			
Vapor Fraction:	1	1			

Design Data:

Material:	Cast Iron
Net Work Requirement (hp):	111.5
ΔPressure (psi):	17.3
Compression Ratio:	4.3

Utilities:

Electricity (kW): 75.0

Comments:

Centrifugal Compressor

Identification:	Item:	*Compressor*			
	Item No.:	*C- 301*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*1,084,345*		C_{BM} ($):	*2,331,342*

Function: Maintains pressure for stream S-310.

Operation: Continuous

	S-310 *Inlet*	*S-311* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	22,481	22,481			
Volumetric Flow (ft^3/hr):	774,892	262,832			
Component Flows (lb/hr):					
O_2	2	2			
H_2	0	0			
N_2	309	309			
Ammonia	54	54			
H_2O	22,113	22,113			
CO_2	3	3			
MPDA	0	0			
3-methylpiperidine	0	0			
3-picoline	0	0			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	387	887			
Pressure (psi):	14.5	68			
Vapor Fraction:	1	1			

Design Data:

Material:	Cast Iron
Net Work Requirement (hp):	2253.0
ΔPressure (psi):	17.3
Compression Ratio:	4.7

Utilities:

Electricity (kW):	1563.1

Comments:

Distillation Tower

Identification:	Item:	*Distillation*		
	Item No.:	*D-101*	Date:	*4/10/13*
	No. Required:	*1*	By:	*JS/AC/PB/AL*
	C_p ($):	*967,255*	C_{BM} ($):	*4,023,779*

Function: Separates MPDA from ammonia and 3-methylpiperidine for recycling.

Operation: Continuous

	S-106 Inlet	*Overhead S-107 Outlet*	*Bottoms S-108 Outlet*		
Materials Handled:					
Total Flow (lb/hr):	3,340	3,307	33		
Volumetric Flow (ft^3/hr):	8,707	29,720	0.7		
Component Flows (lb/hr):					
O_2	0	0	0		
H_2	0	0	0		
N_2	0	0	0		
Ammonia	485	485	Trace		
H_2O	0	0	0		
CO_2	0	0	0		
MPDA	33	Trace	33		
3-methylpiperidine	2,822	2,822	Trace		
3-picoline	0	0	0		
3-cyanopyridine	0	0	0		
Niacinamide	0	0	0		
Temperature (°F):	581	266	379		
Pressure (psi):	71.6	14.7	14.7		
Vapor Fraction:	1	1	<0.001		

Design Data:

Type:	Pressure Vessel
Material:	Carbon Steel
Length (ft):	20.0
Diameter (ft):	1.0
Number of stages:	40

Utilities:

Cooling Water (lb/hr):	231,886
450 psi Steam (lb/hr):	5,304

Comments: * cost reflects emtire unit incl. condenser and reboiler

Condenser

Identification:	Item:	*Fixed Tube Sheet Heat Exchanger*			
	Item No.:	*D-101-condenser*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
				C_{BM} ($):	*59,060*

Design Data:

Type:	Heat Exchanger		Tube	
Refux Ratio:	1		Number of tubes:	52
$T_{h,i}$ (°F):	306	Stage 2	Length (ft):	20
$T_{h,o}$ (°F):	266	Stage 1 / S-107	D_o (in):	1
Total heat duty (MMBtu/hr):	-6.9		Shell	
Material:	Carbon Steel		Length (ft):	20
			D (in):	12
			Number of baffles:	16

Reboiler

Identification:	Item:	*U-tube kettle vaporizer*			
	Item No.:	*D-101-reboiler*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
				C_{BM} ($):	*85,980*

Design Data:

Type:	Heat Exchanger		Tube	
			Number of tubes:	176
$T_{c,i}$ (°F):	318	Stage 40	Length (ft):	20
$T_{c,o}$ (°F):	402	S-108	D_o (in):	1
Tube side h (Btu/hr-ft^2):	1000		Shell	
Shell side h (Btu/hr-ft^2):	200		Length (ft):	13
Total heat transfer A (ft^2):	143		D (in):	21
Total heat duty (MMBtu/hr):	6.4		Number of baffles:	9
Material:	Carbon Steel			

Decolorizer

Identification:	Item:	*Decolorizing unit*		
	Item No.:	*DC-301*	Date:	*4/10/13*
	No. Required:	*1*	By:	*JS/AC/PB/AL*
	C_p ($):	*38,089*	C_{BM} ($):	*149,787*

Function: Removes color from the niacin product.

Operation: Continuous

	S-302 *Inlet*	*S-304* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	25,619	25,619			
Volumetric Flow (ft^3/hr):	465	465			
Component Flows (lb/hr):					
O_2	0.02	0.02			
H_2	Trace	Trace			
N_2	0.002	0.002			
Ammonia	54	54			
H_2O	22,113	22,113			
CO_2	0.4	0.4			
MPDA	0.002	0.002			
3-methylpiperidine	27	27			
3-picoline	23	23			
3-cyanopyridine	29	29			
Niacinamide	3,372	3,372			
Temperature (°F):	77	77			
Pressure (psi):	25	20			
Vapor Fraction:	<0.001	<0.001			

Design Data:

Material:	Carbon steel
Diameter (ft):	4.0
Length (ft):	15.9
Volume (ft^3):	199
Residence Time (min):	10

Utilities:

Comments:

Continuous Turbo-Tray Dryer

Identification:

Item:	*Dryer*		
Item No.:	*DR-301*	Date:	*4/10/13*
No. Required:	*1*	By:	*JS/AC/PB/AL*
C_p ($):	*804,369*	C_{BM} ($):	*1,657,000*

Function: Dries off ammonia and water, leaving a dry powdered form of niacinamide product

Operation: Continuous

	Inlet (S-309)	*Inlet (S-315)*	*Inlet (S-307)*	*Outlet (S-310)*	*Outlet (1-316)*
Materials Handled:					
Total Flow (lb/hr):	31	283	25,619	22,481	3,452
Volumetric Flow (ft^3/hr):	517	1,104	380,573	774,892	44
Component Flows (lb/hr):					
O_2	0	2	0.2	2	0
H_2	0	0	0	0	0
N_2	31	278	0.002	309	0
Ammonia	0	0.03	54	54	0
H_2O	0	0.2	22,113	22,113	0
CO_2	0	3	0.4	3	0
MPDA	0	0	0.002	0	0.002
3-methylpiperidine	0	0	27	0	27
3-picoline	0	0	23	0	23
3-cyanopyridine	0	0	29	0	29
Niacinamide	0	0	3372	0	3372
Temperature (°F):	392	32	392	387	387
Pressure (psi):	19.5	48	29.9	14.5	14.5
Vapor Fraction:	1	1	1	1	0

Design Data:

Evaporation Rate (lb/hr):	650.0
Material:	Stainless steel
Diameter (ft):	20
Height (ft):	23

Utilities:

Comments:

Vapor Liquid Separator

Identification:	Item: *Flash*				
	Item No.: *F-201*			Date: *4/10/13*	
	No. Required: *1*			By: *JS/AC/PB/AL*	
	C_p ($): *128,760*			C_{BM} ($): *535,640*	
Function: Separates O2, H2 and N2 from ammonia, water, niacinamide and the remaining heavy components in the bottoms.					
Operation: Continuous					
	S-227 Inlet	*Overhead S-228 Outlet*	*Bottoms S-229 Outlet*		
Materials Handled:					
Total Flow (lb/hr):	5,795	145	5,650		
Volumetric Flow (ft^3/hr):	917	1,563	75		
Component Flows (lb/hr):					
O_2	136	135	0.2		
H_2	0	0	0		
N_2	0.4	0.4	Trace		
Ammonia	0.08	0.001	0.08		
H_2O	2,199	0.5	2,198		
CO_2	7	7	0.3		
MPDA	0.002	Trace	0.002		
3-methylpiperidine	28	1	27		
3-picoline	24	0.3	23		
3-cyanopyridine	29	0.03	29		
Niacinamide	3372	Trace	3372		
Temperature (°F):	32	32	32		
Pressure (psi):	27.6	15	15		
Vapor Fraction:	0.029	1	0		

Design Data:

Type:	Pressure Vessel
Material:	Carbon Steel
Length (ft):	12.0
Diameter (ft):	3.0

Utilities:

Comments:

Vapor Liquid Separator

Identification:	Item:	*Flash*			
	Item No.:	*F-301*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*115,273*		C_{BM} ($):	*479,535*

Function: Separates 3-methylpiperidine, 3-picoline and 3-cyanopyridine from stream O_2, H_2, N_2, H_2O and CO_2 effluent

Operation: Continuous

	S-312 *Inlet*	*Overhead S-313* *Outlet*	*Bottoms S-317* *Outlet*		
Materials Handled:					
Total Flow (lb/hr):	22,481	315	22,166		
Volumetric Flow (ft^3/hr):	1,365	1,016	349		
Component Flows (lb/hr):					
O_2	2	2	0.001		
H_2	0	0	0		
N_2	309	309	0.002		
Ammonia	54	0.03	54		
H_2O	22,113	0.2	22,113		
CO_2	3	3	0.02		
MPDA	0	0	0		
3-methylpiperidine	0	0	0		
3-picoline	0	0	0		
3-cyanopyridine	0	0	0		
Niacinamide	0	0	0		
Temperature (°F):	32	32	32		
Pressure (psi):	58	58	58		
Vapor Fraction:	0.009	1	0		

Design Data:

Type:	Pressure Vessel
Material:	Carbon Steel
Length (ft):	12.0
Diameter (ft):	4.0

Utilities:

Comments:

Heat Exchanger

Identification:	Item: *Floating head shell-and-tube*		
	Item No.: *HX-101*	Date:	*4/10/13*
	No. Required: *1*	By:	*JS/AC/PB/AL*
	C_p (\$): *76,656*	C_{BM} (\$):	*243,001*

Function: Preheater for MPDA feed to first reactor.

Operation: Continuous

	S-103 *Cold In*	*S-104* *Cold Out*			
Materials Handled:					
Total Flow (lb/hr):	3,340	3,340			
Volumetric Flow (ft^3/hr):	55	8,642			
Component Flows (lb/hr):					
O_2	0	0			
H_2	0	0			
N_2	0	0			
Ammonia	Trace	Trace			
H_2O	0	0			
CO_2	0	0			
MPDA	3,340	3,341			
3-methylpiperidine	Trace	Trace			
3-picoline	0	0			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	81	527			
Pressure (psi):	43.5	33.5			
Vapor Fraction:	0	1			

Design Data:

Q (Btu/hr):	1,468,101	$T_{h,i}$ (°F):	712.9
U_0 (Btu/hr-ft^2-°F):	175.0	$T_{h,o}$ (°F):	400.0
U_i (Btu/hr-ft^2-°F):	200.0	$T_{c,i}$ (°F):	81.0
A_0 (ft^2):	143	$T_{c,o}$ (°F):	527.0
Material:	Carbon Steel	ΔT_{lm} (°F):	246.5

Utilities:

Dowtherm A (MMBTU/hr):	1.47
Dowtherm A (lb/hr):	5,872

Comments: Hot stream is on the shell side and cold stream is on the tube side.

Heat Exchanger

Identification: Item:	*Floating head shell-and-tube*		
Item No.:	*HX-102*	Date:	*4/10/13*
No. Required:	*1*	By:	*JS/AC/PB/AL*
C_p ($):	*74,697*	C_{BM} ($):	*236,789*

Function: Preheater for feed to second reactor.

Operation: Continuous

	S-110 *Cold In*	*S-111* *Cold Out*			
Materials Handled:					
Total Flow (lb/hr):	3,307	3,307			
Volumetric Flow (ft^3/hr):	6,848	9,682			
Component Flows (lb/hr):					
O_2	0	0			
H_2	0	0			
N_2	0	0			
Ammonia	485	485			
H_2O	0	0			
CO_2	0	0			
MPDA	0.002	0.002			
3-methylpiperidine	2822	2822			
3-picoline	0	0			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	393	554			
Pressure (psi):	72.5	62.5			
Vapor Fraction:	1	1			

Design Data:

Q (Btu/hr):	292,947	$T_{h,i}$ (°F):	712.9
U_0 (Btu/hr-ft^2-°F):	175	$T_{h,o}$ (°F):	400.0
U_i (Btu/hr-ft^2-°F):	100	$T_{c,i}$ (°F):	393.0
A_0 (ft^2):	104	$T_{c,o}$ (°F):	554.0
Material:	Carbon steel	ΔT_{lm} (°F):	48.6

Utilities:

Dowtherm A (MMBTU/hr):	0.29
Dowtherm A (lb/hr):	1172

Comments: Hot stream is on the shell side and cold stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*				
	Item No.:	*HX-201*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*133,947*			C_{BM} ($):	*424,612*

Function: Heater for feed to third reactor.

Operation: Continuous

	S-203A *Cold In*	*S-203* *Cold Out*			
Materials Handled:					
Total Flow (lb/hr):	3,307	3,307			
Volumetric Flow (ft^3/hr):	47,740	41,773			
Component Flows (lb/hr):					
O_2	0	0			
H_2	Trace	Trace			
N_2	0	0			
Ammonia	Trace	475			
H_2O	0	0			
CO_2	0	0			
MPDA	0.002	0			
3-methylpiperidine	28	0			
3-picoline	2,622	1			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	366	224			
Pressure (psi):	40	170			
Vapor Fraction:	<0.001	<0.001			

Design Data:

Q (Btu/hr):	2,600,308	$T_{h,i}$ (°F):	712.9
U_0 (Btu/hr-ft^2-°F):	143	$T_{h,o}$ (°F):	400.0
U_i (Btu/hr-ft^2-°F):	200	$T_{c,i}$ (°F):	224.0
A_0 (ft^2):	209	$T_{c,o}$ (°F):	366.0
Material:	Carbon steel	ΔT_{lm} (°F):	251.9

Utilities:

Dowtherm A (MMBTU/hr):	2.60
Dowtherm A (lb/hr):	10400

Comments: Cool stream is on the shell side and hot stream is on the tube side.

Heat Exchanger						
Identification:	Item:	*Floating head shell-and-tube*				
	Item No.:	*HX-202A*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*104,322*			C_{BM} ($):	*330,700*
Function: Cooler for feed to first CSTR.						
Operation: Continuous						
	S-205	*S-206A*				
	Hot In	*Hot Out*				
Materials Handled:						
Total Flow (lb/hr):	5,795	5,795				
Volumetric Flow (ft^3/hr):	72,571	1,245				
Component Flows (lb/hr):						
O_2	136	136				
H_2	0	0				
N_2	0.4	0.4				
Ammonia	0.08	0.08				
H_2O	2,696	2,696				
CO_2	7	7				
MPDA	0.002	0.002				
3-methylpiperidine	28	28				
3-picoline	24	24				
3-cyanopyridine	2,904	2,904				
Niacinamide	0	0				
Temperature (°F):	626	100				
Pressure (psi):	29.1	24.1				
Vapor Fraction:	1	0.025				
Design Data:						
Q (Btu/hr):	4,376,826			$T_{h,i}$ (°F):	626.0	
U_0 (Btu/hr-ft^2-°F):	1019.0			$T_{h,o}$ (°F):	100.0	
U_i (Btu/hr-ft^2-°F):	1,053			$T_{c,i}$ (°F):	90.0	
A_0 (ft^2):	146			$T_{c,o}$ (°F):	120.0	
Material:	Carbon Steel			ΔT_{lm} (°F):	126.4	
Utilities:						
Cooling water (lb/hr):	146,388					
Comments: Cold stream is on the shell side and hot stream is on the tube side.						

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*			
	Item No.:	*HX-202B*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*77,117*		C_{BM} ($):	*244,462*

Function: Cooler for feed to first CSTR.

Operation: Continuous

	S-206A	*S-206*			
	Hot In	*Hot Out*			
Materials Handled:					
Total Flow (lb/hr):	5,795	5,795			
Volumetric Flow (ft^3/hr):	1,245	1,457			
Component Flows (lb/hr):					
O_2	136	136			
H_2	0	0			
N_2	0.4	0.4			
Ammonia	0.08	0.08			
H_2O	2,696	2,696			
CO_2	7	7			
MPDA	0.002	0.002			
3-methylpiperidine	28	28			
3-picoline	24	24			
3-cyanopyridine	2,904	2,904			
Niacinamide	0	0			
Temperature (°F):	100	77			
Pressure (psi):	24.1	19.1			
Vapor Fraction:	0.025	0.025			

Design Data:

Q (Btu/hr):	-951,843	$T_{h,i}$ (°F):	625.0
U_0 (Btu/hr-ft^2-°F):	469.0	$T_{h,o}$ (°F):	77.0
U_i (Btu/hr-ft^2-°F):	1053	$T_{c,i}$ (°F):	-14.0
A_0 (ft^2):	224	$T_{c,o}$ (°F):	-11.7
Material:	Carbon Steel	ΔT_{lm} (°F):	280.5

Utilities:

Refrigeration (ton/day): 26,057

Comments: Cold stream is on the shell side and hot stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*			
	Item No.:	*HX-203*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*57,636*		C_{BM} ($):	*182,707*

Function: Cooler for feed to second CSTR.

Operation: Continuous

	S-212 *Hot In*	*S-213* *Hot Out*			
Materials Handled:					
Total Flow (lb/hr):	5,795	5,795			
Volumetric Flow (ft^3/hr):	950	1,405			
Component Flows (lb/hr):					
O_2	136	136			
H_2	0	0			
N_2	0.4	0.4			
Ammonia	0.08	0.08			
H_2O	2,199	2,199			
CO_2	7	7			
MPDA	0.002	0.002			
3-methylpiperidine	28	28			
3-picoline	24	24			
3-cyanopyridine	2,904	2,904			
Niacinamide	0	0			
Temperature (°F):	79	77			
Pressure (psi):	29.6	19.6			
Vapor Fraction:	0.029	0.029			

Design Data:

Q (Btu/hr):	-7,284	$T_{h,i}$ (°F):	79.0
U_0 (Btu/hr-ft^2-°F):	303.0	$T_{h,o}$ (°F):	77.0
U_i (Btu/hr-ft^2-°F):	250	$T_{c,i}$ (°F):	-14.0
A_0 (ft^2):	5.23	$T_{c,o}$ (°F):	-11.7
Material:	Carbon Steel	ΔT_{lm} (°F):	90.9

Utilities:

Refrigeration (ton/day): 199

Comments: Cold stream is on the shell side and hot stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*		
	Item No.:	*HX-204*	Date:	*4/10/13*
	No. Required:	*1*	By:	*JS/AC/PB/AL*
	C_p ($):	*57,636*	C_{BM} ($):	*182,707*

Function: Cooler for feed to third CSTR.

Operation: Continuous

	S-219	*S-220*			
	Hot In	*Hot Out*			
Materials Handled:					
Total Flow (lb/hr):	5,795	5,795			
Volumetric Flow (ft^3/hr):	1,245	1,457			
Component Flows (lb/hr):					
O_2	136	136			
H_2	0	0			
N_2	0.4	0.4			
Ammonia	0.08	0.08			
H_2O	2,199	2,199			
CO_2	7	7			
MPDA	0.002	0.002			
3-methylpiperidine	28	28			
3-picoline	24	24			
3-cyanopyridine	2,904	2,904			
Niacinamide	0	0			
Temperature (°F):	79	77			
Pressure (psi):	30.1	20.1			
Vapor Fraction:	0.029	0.029			

Design Data:

Q (Btu/hr):	-6,495	$T_{h,i}$ (°F):	79.0
U_0 (Btu/hr-ft^2-°F):	303.0	$T_{h,o}$ (°F):	77.0
U_i (Btu/hr-ft^2-°F):	250	$T_{c,i}$ (°F):	-14.0
A_0 (ft^2):	5.23	$T_{c,o}$ (°F):	-11.7
Material:	Carbon Steel	ΔT_{lm} (°F):	90.9

Utilities:

Refrigeration (ton/day): 178

Comments: Cold stream is on the shell side and hot stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*			
	Item No.:	*HX-205*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*72,622*		C_{BM} ($):	*230,211*

Function: Cooler for feed to first flash vessel.

Operation: Continuous

	S-226	*S-227*			
	Hot In	*Hot Out*			
Materials Handled:					
Total Flow (lb/hr):	5,795	5,795			
Volumetric Flow (ft^3/hr):	761	917			
Component Flows (lb/hr):					
O_2	136	136			
H_2	0	0			
N_2	0.4	0.4			
Ammonia	0.08	0.08			
H_2O	2,199	2,199			
CO_2	7	7			
MPDA	Trace	Trace			
3-methylpiperidine	28	28			
3-picoline	24	24			
3-cyanopyridine	29	29			
Niacinamide	3372	3372			
Temperature (°F):	79	32			
Pressure (psi):	37.6	27.6			
Vapor Fraction:	0.029	0.029			

Design Data:

Q (Btu/hr):	-185,853	$T_{h,i}$ (°F):	79.0
U_0 (Btu/hr-ft^2-°F):	469.0	$T_{h,o}$ (°F):	32.0
U_i (Btu/hr-ft^2-°F):	250	$T_{c,i}$ (°F):	-14.0
A_0 (ft^2):	28.5	$T_{c,o}$ (°F):	-11.7
Material:	Carbon Steel	ΔT_{lm} (°F):	65.9

Utilities:

Refrigeration (ton/day): 5,064

Comments: Cold stream is on the shell side and hot stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*		
	Item No.:	*HX-206*	Date:	*4/10/13*
	No. Required:	*1*	By:	*JS/AC/PB/AL*
	C_p ($):	*53,371*	C_{BM} ($):	*169,187*

Function: Heater for S-230.

Operation: Continuous

	S-230 *Cold In*	*S-231* *Cold Out*
Materials Handled:		
Total Flow (lb/hr):	5,650	5,650
Volumetric Flow (ft^3/hr):	75	77
Component Flows (lb/hr):		
O_2	0.2	0.2
H_2	0	0
N_2	Trace	Trace
Ammonia	0.08	0.08
H_2O	2,199	2,199
CO_2	0.3	0.3
MPDA	0.002	0.002
3-methylpiperidine	27	27
3-picoline	23	23
3-cyanopyridine	29	29
Niacinamide	3,372	3,372
Temperature (°F):	32	90
Pressure (psi):	45	35
Vapor Fraction:	0	0

Design Data:

Q (Btu/hr):	223,486	$T_{h,i}$ (°F):	100.0
U_0 (Btu/hr-ft^2-°F):	303.0	$T_{h,o}$ (°F):	90.0
U_i (Btu/hr-ft^2-°F):	1000	$T_{c,i}$ (°F):	32.2
A_0 (ft^2):	5.96	$T_{c,o}$ (°F):	90.0
Material:	Carbon Steel	ΔT_{lm} (°F):	27.2

Utilities:

100 °F Water (lb/hr): 185

Comments: Hot stream is on the shell side and cold stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*			
	Item No.:	*HX-301*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*66,282*		C_{BM} ($):	*210,113*

Function: Preheater for feed to decolorizing unit.

Operation: Continuous

	S-301 *Cold In*	*S-302* *Cold Out*			
Materials Handled:					
Total Flow (lb/hr):	25,619	25,619			
Volumetric Flow (ft^3/hr):	433	465			
Component Flows (lb/hr):					
O_2	0.2	1.2			
H_2	Trace	Trace			
N_2	0.002	0.002			
Ammonia	54	54			
H_2O	22,113	22,113			
CO_2	0.4	0.4			
MPDA	0.002	0.002			
3-methylpiperidine	27	27			
3-picoline	23	23			
3-cyanopyridine	29	29			
Niacinamide	3372	3372			
Temperature (°F):	31	77			
Pressure (psi):	35	25			
Vapor Fraction:	<0.001	<0.001			

Design Data:

Q (Btu/hr):	1,238,182	$T_{h,i}$ (°F):	100.0
U_0 (Btu/hr-ft^2-°F):	1053.0	$T_{h,o}$ (°F):	90.0
U_i (Btu/hr-ft^2-°F):	1000	$T_{c,i}$ (°F):	31.0
A_0 (ft^2):	20.6	$T_{c,o}$ (°F):	77.0
Material:	Carbon Steel	ΔT_{lm} (°F):	38.2

Utilities:

100 °F Water (lb/hr): 1,021

Comments: Hot stream is on the shell side and cold stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*			
	Item No.:	*HX-302*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*123,457*		C_{BM} ($):	*391,359*

Function: Preheater for slurry feed to spray dryer.

Operation: Continuous

	S-306 *Cold In*	*S-307* *Cold Out*
Materials Handled:		
Total Flow (lb/hr):	25,619	25,619
Volumetric Flow (ft^3/hr):	400	380,573
Component Flows (lb/hr):		
O_2	0.2	0.2
H_2	0	0
N_2	0.002	0.002
Ammonia	54	54
H_2O	22,113	22,113
CO_2	0.4	0.4
MPDA	0.002	0.002
3-methylpiperidine	27	27
3-picoline	23	23
3-cyanopyridine	29	29
Niacinamide	3,372	3,372
Temperature (°F):	77	392
Pressure (psi):	39.9	29.9
Vapor Fraction:	0	1

Design Data:

Q (Btu/hr):	28,922,227	$T_{h,i}$ (°F):	460.0
U_0 (Btu/hr-ft^2-°F):	526.0	$T_{h,o}$ (°F):	460.0
U_i (Btu/hr-ft^2-°F):	1000	$T_{c,i}$ (°F):	77.0
A_0 (ft^2):	948	$T_{c,o}$ (°F):	392.0
Material:	Carbon Steel	ΔT_{lm} (°F):	182.2

Utilities:

450 psi Steam (lb/hr): 24,002

Comments: Hot stream is on the shell side and cold stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*			
	Item No.:	*HX-303*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*56,829*		C_{BM} ($):	*180,149*

Function: Preheater for N_2 feed to spray dryer.

Operation: Continuous

	S-308 *Cold In*	*S-309* *Cold Out*			
Materials Handled:					
Total Flow (lb/hr):	31	31			
Volumetric Flow (ft^3/hr):	215	517			
Component Flows (lb/hr):					
O_2	0	0			
H_2	0	0			
N_2	31	31			
Ammonia	0	0			
H_2O	0	0			
CO_2	0	0			
MPDA	0	0			
3-methylpiperidine	0	0			
3-picoline	0	0			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	77	392			
Pressure (psi):	29.5	19.5			
Vapor Fraction:	1	1			

Design Data:

Q (Btu/hr):	2,431	$T_{h,i}$ (°F):	460.0
U_0 (Btu/hr-ft^2-°F):	30.0	$T_{h,o}$ (°F):	460.0
U_i (Btu/hr-ft^2-°F):	1000	$T_{c,i}$ (°F):	77.0
A_0 (ft^2):	5.24	$T_{c,o}$ (°F):	392.0
Material:	Carbon Steel	ΔT_{lm} (°F):	182.2

Utilities:

450 psi Steam (lb/hr): 2

Comments: Hot stream is on the shell side and cold stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*		
	Item No.:	*HX-304A*	Date:	*4/10/13*
	No. Required:	*1*	By:	*JS/AC/PB/AL*
	C_p ($):	*253,139*	C_{BM} ($):	*802,450*

Function: Cooler for feed to third flash vessel (F-301).

Operation: Continuous

	S-311 *Hot In*	*S-312A* *Hot Out*			
Materials Handled:					
Total Flow (lb/hr):	22,481	22,481			
Volumetric Flow (ft^3/hr):	262,833	1,440			
Component Flows (lb/hr):					
O_2	2	2			
H_2	0	0			
N_2	309	309			
Ammonia	54	54			
H_2O	22,113	22,113			
CO_2	3	3			
MPDA	0	0			
3-methylpiperidine	0	0			
3-picoline	0	0			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	887	100			
Pressure (psi):	68	63			
Vapor Fraction:	1	0.009			

Design Data:

Q (Btu/hr):	-32,862,364	$T_{h,i}$ (°F):	887.0
U_0 (Btu/hr-ft^2-°F):	265.0	$T_{h,o}$ (°F):	100.0
U_i (Btu/hr-ft^2-°F):	1053	$T_{c,i}$ (°F):	90.0
A_0 (ft^2):	1411	$T_{c,o}$ (°F):	120.0
Material:	Stainless Steel	ΔT_{lm} (°F):	174.4

Utilities:

Cooling water (lb/hr): 1,099,120

Comments: Cold stream is on the shell side and hot stream is on the tube side.

Heat Exchanger

Identification:	Item:	*Floating head shell-and-tube*			
	Item No.:	*HX-304B*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*88,414*		C_{BM} ($):	*280,273*

Function: Cooler for feed to third flash vessel (F-301).

Operation: Continuous

	S-312A *Hot In*	*S-312* *Hot Out*			
Materials Handled:					
Total Flow (lb/hr):	22,481	22,481			
Volumetric Flow (ft^3/hr):	1,440	1,365			
Component Flows (lb/hr):					
O_2	2	2			
H_2	0	0			
N_2	309	309			
Ammonia	54	54			
H_2O	22,113	22,113			
CO_2	3	3			
MPDA	0	0			
3-methylpiperidine	0	0			
3-picoline	0	0			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	100	32			
Pressure (psi):	63	58			
Vapor Fraction:	0.009	0.009			

Design Data:

Q (Btu/hr):	-1,752,229	$T_{h,i}$ (°F):	100.0
U_0 (Btu/hr-ft^2-°F):	469.0	$T_{h,o}$ (°F):	32.0
U_i (Btu/hr-ft^2-°F):	250	$T_{c,i}$ (°F):	-14.0
A_0 (ft^2):	242	$T_{c,o}$ (°F):	-11.7
Material:	Carbon Steel	ΔT_{lm} (°F):	74.1

Utilities:

Refrigeration (ton/day): 47,967

Comments: Cold stream is on the shell side and hot stream is on the tube side.

Neutralizer

Identification:	Item:	*Neutralizer*				
	Item No.:	*N-301*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*45,900*			C_{BM} ($):	*142,736*

Function: Neutralizes S-304 in buffer solution forming a salt and then a mixed solution.

Operation: Continuous

	S-304 *Inlet*	*S-305* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	25,619	25,619			
Volumetric Flow (ft^3/hr):	496	556			
Component Flows (lb/hr):					
O_2	0.2	0.2			
H_2	Trace	0			
N_2	0.002	0.002			
Ammonia	54	54			
H_2O	22,113	22,113			
CO_2	0.4	0.4			
MPDA	0.004	0.004			
3-methylpiperidine	27	27			
3-picoline	23	23			
3-cyanopyridine	29	29			
Niacinamide	3,372	3,372			
Ammonium Nicotinate	0	0			
Temperature (°F):	77	77			
Pressure (psi):	20	15			
Vapor Fraction:	<0.001	<0.001			

Design Data:

Material:	Carbon Steel
Diameter (ft):	3.5
Length (ft):	14.2
Residence time (hr):	0.167
Volume (ft^3):	140

Utilities:

Comments: Modeled as vertical pressure vessel with turbine agitators

Centrifugal Pump						
Identification:	Item:	*Pump*				
	Item No.:	*P-101*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*30,547*			C_{BM} ($):	*100,806*
Function: MPDA feed pump.						
Operation: Continuous						
	S-101	*S-102*				
	Inlet	*Outlet*				
Materials Handled:						
Total Flow (lb/hr):	3,307	3,307				
Volumetric Flow (ft^3/hr):	54	54				
Component Flows (lb/hr):						
O_2	0	0				
H_2	0	0				
N_2	0	0				
Ammonia	0	0				
H_2O	0	0				
CO_2	0	0				
Niacinamide	0	0				
MPDA	3,307	3,307				
3-methylpiperidine	0	0				
3-picoline	0	0				
3-cyanopyridine	0	0				
Ammonium Nicotinate	0	0				
Temperature (°F):	77	77				
Pressure (psi):	14.5	43.5				
Vapor Fraction:	0	0				
Design Data:						
Flow Rate (gpm):	7.39					
ΔP (psi):	29.0					
Pump Head (ft):	68.2					
Material:	Cast Steel					
Speed:	3600 rpm					
P_c (hp):	0.5					
Efficiency:	0.296					
Utilities:						
Electricity (kW):	0.3					
Comments:						

Centrifugal Pump

Identification:	Item:	*Pump*				
	Item No.:	*P-102*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*30,432*			C_{BM} ($):	*100,426*

Function: MPDA recycle stream pump.

Operation: Continuous

	S-108 *Inlet*	*S-109* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	33	33			
Volumetric Flow (ft^3/hr):	0.7	0.7			
Component Flows (lb/hr):					
O_2	0	0			
H_2	0	0			
N_2	0	0			
Ammonia	Trace	Trace			
H_2O	0	0			
CO_2	0	0			
Niacinamide	0	0			
MPDA	33	33			
3-methylpiperidine	0.002	0.002			
3-picoline	0	0			
3-cyanopyridine	0	0			
Ammonium Nicotinate	0	0			
Temperature (°F):	379	380			
Pressure (psi):	14.5	43.5			
Vapor Fraction:	<0.001	0			

Design Data:

Flow Rate (gpm):	0.093
ΔP (psi):	29.0
Pump Head (ft):	67
Material:	Cast Steel
Speed:	3600 rpm
P_c (hp):	0.125
Efficiency:	0.296

Utilities:

Electricity (kW):	0.003

Comments:

Centrifugal Pump						
Identification:	Item:	*Pump*				
	Item No.:	*P-103*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*41,844*			C_{BM} ($):	*138,085*
Function: Pump water into the ammonia absorption column						
Operation: Continuous						
	S-116 *Inlet*	*S-117* *Outlet*				
Materials Handled:						
Total Flow (lb/hr):	1,200	1,200				
Volumetric Flow (ft^3/hr):	19	19				
Component Flows (lb/hr):						
O_2	0	0				
H_2	0	0				
N_2	0	0				
Ammonia	0	0				
H_2O	1,200	1,200				
CO_2	0	0				
Niacinamide	0	0				
MPDA	0	0				
3-methylpiperidine	0	0				
3-picoline	0	0				
3-cyanopyridine	0	0				
Ammonium Nicotinate	0	0				
Temperature (°F):	90	91				
Pressure (psi):	15	170				
Vapor Fraction:	0	0				
Design Data:						
Flow Rate (gpm):	2.67					
ΔP (psi):	155.0					
Pump Head (ft):	363					
Material:	Cast Steel					
Speed:	3600 rpm					
P_c (hp):	1					
Efficiency:	0.296					
Utilities:						
Electricity (kW):	0.5					
Comments:						

Centrifugal Pump

Identification:	Item:	*Pump*			
	Item No.:	*P-201*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*34,467*		C_{BM} ($):	*113,740*

Function: Pump liquid product from first CSTR to second CSTR

Operation: Continuous

	S-210 *Inlet*	*S-211* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	5,647	5,647			
Volumetric Flow (ft^3/hr):	76	76			
Component Flows (lb/hr):					
O_2	0.3	0.3			
H_2	0	0			
N_2	Trace	Trace			
Ammonia	0.8	0.8			
H_2O	2,196	2,196			
CO_2	0.3	0.3			
Niacinamide	3,372	3,372			
MPDA	0.002	0.002			
3-methylpiperidine	26	26			
3-picoline	23	23			
3-cyanopyridine	29	29			
Ammonium Nicotinate	0	0			
Temperature (°F):	77	77			
Pressure (psi):	14.6	29.6			
Vapor Fraction:	0	0			

Design Data:

Flow Rate (gpm):	10.5
ΔP (psi):	15.0
Pump Head (ft):	29.2
Material:	Cast Steel
Speed:	3600 rpm
P_c (hp):	0.33
Efficiency:	0.296

Utilities:

Electricity (kW):	0.2

Comments: Similar to P-202

Centrifugal Pump						
Identification:	Item:	*Pump*				
	Item No.:	*P-202*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*34,467*			C_{BM} ($):	*113,740*
Function: Pump liquid product from second CSTR to third CSTR						
Operation: Continuous						
	S-217	*S-218*				
	Inlet	*Outlet*				
Materials Handled:						
Total Flow (lb/hr):	5,647	5,647				
Volumetric Flow (ft^3/hr):	76	76				
Component Flows (lb/hr):						
O_2	0.3	0.3				
H_2	0	0				
N_2	Trace	Trace				
Ammonia	0.8	0.8				
H_2O	2,196	2,196				
CO_2	0.3	0.3				
Niacinamide	3,372	3,372				
MPDA	0.002	0.002				
3-methylpiperidine	26	26				
3-picoline	23	23				
3-cyanopyridine	29	29				
Ammonium Nicotinate	0	0				
Temperature (°F):	77	77				
Pressure (psi):	15.1	30.1				
Vapor Fraction:	0	0				
Design Data:						
Flow Rate (gpm):	10.5					
ΔP (psi):	15.0					
Pump Head (ft):	29.2					
Material:	Cast Steel					
Speed:	3600 rpm					
P_c (hp):	0.33					
Efficiency:	0.296					
Utilities:						
Electricity (kW):	0.2					
Comments: Similar to P-201						

Centrifugal Pump						
Identification:	Item:	*Pump*				
	Item No.:	*P-203*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*34,467*			C_{BM} ($):	*113,740*
Function: Pump liquid product from third CSTR to flash vessel						
Operation: Continuous						
	S-224	*S-225*				
	Inlet	*Outlet*				
Materials Handled:						
Total Flow (lb/hr):	5,647	5,647				
Volumetric Flow (ft^3/hr):	76	76				
Component Flows (lb/hr):						
O_2	0.3	0.3				
H_2	0	0				
N_2	Trace	Trace				
Ammonia	0.8	0.8				
H_2O	2,196	2,196				
CO_2	0.3	0.3				
Niacinamide	3,372	3,372				
MPDA	0.002	0.002				
3-methylpiperidine	26	26				
3-picoline	23	23				
3-cyanopyridine	29	29				
Ammonium Nicotinate	0	0				
Temperature (°F):	77	77				
Pressure (psi):	15.6	45.6				
Vapor Fraction:	0	0				
Design Data:						
Flow Rate (gpm):	10.5					
ΔP (psi):	30.0					
Pump Head (ft):	58.5					
Material:	Cast Steel					
Speed:	3600 rpm					
P_c (hp):	0.75					
Efficiency:	0.296					
Utilities:						
Electricity (kW):	0.4					
Comments:						

Centrifugal Pump

Identification:	Item:	*Pump*			
	Item No.:	*P-204*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*31,239*		C_{BM} ($):	*103,088*

Function: S-229 pump.

Operation: Continuous

	S-229 *Inlet*	*S-230* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	5,650	5,650			
Volumetric Flow (ft^3/hr):	75	75			
Component Flows (lb/hr):					
O_2	0.2	0.2			
H_2	0	0			
N_2	Trace	Trace			
Ammonia	0.08	0.08			
H_2O	2,198	2,198			
CO_2	0.3	0.3			
Niacinamide	3,372	3,372			
MPDA	0.002	0.002			
3-methylpiperidine	27	27			
3-picoline	23	23			
3-cyanopyridine	29	29			
Ammonium Nicotinate	29	29			
Temperature (°F):	32	32			
Pressure (psi):	15	45			
Vapor Fraction:	0	0			

Design Data:

Flow Rate (gpm):	10.3
ΔP (psi):	30.0
Pump Head (ft):	57.3
Material:	Cast Steel
Speed:	3600 rpm
P_c (hp):	0.75
Efficiency:	0.296

Utilities:

Electricity (kW):	0.4

Comments:

Centrifugal Pump						
Identification:	Item:	*Pump*				
	Item No.:	*P-301*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*36,541*			C_{BM} ($):	*120,587*
Function: S-305 pump.						
Operation: Continuous						
	S-305 Inlet	*S-306 Outlet*				
Materials Handled:						
Total Flow (lb/hr):	25,619	25,619				
Volumetric Flow (ft^3/hr):	556	400				
Component Flows (lb/hr):						
O_2	0.02	0.02				
H_2	0	0				
N_2	0.002	0.002				
Ammonia	54	54				
H_2O	22,113	22,113				
CO_2	0.4	0.4				
Niacinamide	3,372	3,372				
MPDA	0.002	0.002				
3-methylpiperidine	28	28				
3-picoline	23	23				
3-cyanopyridine	29	29				
Ammonium Nicotinate	0	0				
Temperature (°F):	77	77				
Pressure (psi):	15	40				
Vapor Fraction:	<0.001	0				
Design Data:						
Flow Rate (gpm):	54.8					
ΔP (psi):	25.0					
Pump Head (ft):	56.2					
Material:	Cast Steel					
Speed:	3600 rpm					
P_c (hp):	2					
Efficiency:	0.44					
Utilities:						
Electricity (kW):	1.2					
Comments:						

Tubular Reactor

Identification:	Item:	*RSTOIC Reactor*				
	Item No.:	*R-101*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*810,184*			C_{BM} ($):	*2,568,283*

Function: Converts MPDA feed to 3-methylpiperidine product

Operation: Continuous

	S-105 *Inlet*	*S-106* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	3,340	3,340			
Volumetric Flow (ft^3/hr):	3,915	8,707			
Component Flows (lb/hr):					
O_2	0	0			
H_2	0	0			
N_2	0	0			
Ammonia	Trace	485			
H_2O	0	0			
CO_2	0	0			
MPDA	3,340	33			
3-methylpiperidine	0.002	2,822			
3-picoline	0	0			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	560	581			
Pressure (psi):	72.5	71.6			
Vapor Fraction:	1	1			

Design Data:

Material:	Stainless Steel
Number of Parallel Tubes:	15
Tube Diameter (in):	6.625
Tube Length (ft):	685.0
Shell Diameter (ft):	1.87
Heat Transfer Area (ft^2):	17,800
Catalyst:	HZSM-5

Utilities:

Cooling Water (lb/hr):	15,118

Comments: Cost as a fixed-head shell-and-tube heat exchanger in modules

Packed-Bed Reactor

Identification:	Item:	*RSTOIC Reactor*			
	Item No.:	*R-102*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*30,713*		C_{BM} ($):	*97,359*

Function: Converts 3-methylpiperidine feed to 3-picoline product

Operation: Continuous

	S-111 *Inlet*	*S-112* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	3,307	3,307			
Volumetric Flow (ft^3/hr):	15,136	76,860			
Component Flows (lb/hr):					
O_2	0	0			
H_2	0	170			
N_2	0	0			
Ammonia	485	485			
H_2O	0	0			
CO_2	0	0			
MPDA	0.002	0.002			
3-methylpiperidine	2,822	28			
3-picoline	0	2,624			
3-cyanopyridine	0	0			
Niacinamide	0	0			
Temperature (°F):	554	554			
Pressure (psi):	62.5	42.2			
Vapor Fraction:	1	1			

Design Data:

Material:	Stainless Steel
Number of Parallel Tubes:	40
Tube Diameter (in):	4.0
Tube Length (ft):	20.0
Shell Diameter (ft):	1.87
Heat Transfer Area (ft^2):	838
Catalyst:	$Pd\text{-}SiO_2/Al_2O_3$

Utilities:

Dowtherm A (MMBTU/hr):	2.6
Dowtherm A (lb/hr):	10,408

Comments: Cost as a fixed-head shell-and-tube heat exchanger in modules

Tubular Reactor					
Identification:	Item:	*RSTOIC Reactor*			
	Item No.:	*R-201*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p ($):	*721,219*		C_{BM} ($):	*2,286,265*
Function: Converts 3-picoline feed to 3-cyanopyridine product					
Operation: Continuous					
	S-203 *Inlet*	*S-204* *Inlet (O_2)*	*S-205* *Outlet*		
Materials Handled:					
Total Flow (lb/hr):	4,314	1,481	5,795		
Volumetric Flow (ft^3/hr):	47,201	6,748	72,571		
Component Flows (lb/hr):					
O_2	0	1,481	136		
H_2	Trace	0	0		
N_2	0	0	0.4		
Ammonia	475	0	0.08		
H_2O	1,186	0	2,696		
CO_2	0	0	7		
MPDA	0.002	0	0.002		
3-methylpiperidine	28	0	28		
3-picoline	2,624	0	24		
3-cyanopyridine	0	0	2,904		
Niacinamide	0	0	0		
Temperature (°F):	626	77	626		
Pressure (psi):	30	39.5	29.1		
Vapor Fraction:	1	1	1		
Design Data:					
Material:	Stainless Steel				
Number of Parallel Tubes:	2,000				
Tube Diameter (in):	1.8				
Tube Length (ft):	42.0				
Shell Diameter (ft):	1.87				
Heat Transfer Area (ft^2):	39,580				
Catalyst:	V_2O_5, TiO_2, ZrO_2 in a 1:3:8 molar ratio and MoO_3 as 1.15 wt% based on V_2O_5				
Utilities:					
Cooling Water (lb/hr):	196,694				
Comments: Cost as a fixed-head shell-and-tube heat exchanger in modules					

Stirred-Tank Reactors in Series					
Identification:	Item:	*RSTOIC Reactor*			
	Item No.:	*R-202A,B,C*		Date:	*4/10/13*
	No. Required:	*3*		By:	*JS/AC/PB/AL*
	C_p ($):	*268,719*		C_{BM} ($):	*918,160**
Function: Converts feed 3-cyanopyridine to niacinamide product					
Operation: Semi-continuous					
	S-206, 213, 220 *Inlet*	*S-207, 214, 221* *Outlet*			
Materials Handled:					
Total Flow (lb/hr):	5,795	5,795			
Volumetric Flow (ft^3/hr):	1,457	1,878			
Component Flows (lb/hr):					
O_2	136	136			
H_2	0	0			
N_2	0.4	0.4			
Ammonia	0.08	0.08			
H_2O	2,696	2,199			
CO_2	7	7			
MPDA	0.002	0.002			
3-methylpiperidine	28	28			
3-picoline	24	24			
3-cyanopyridine	2,904	29			
Niacinamide	0	3,372			
Temperature (°F):	77	77			
Pressure (psi):	19.1	14.6			
Vapor Fraction:	0.025	0.03			
Design Data:					
Material:	Carbon Steel (SA-285 Grade C)				
Stirrer Speed (rpm):	110				
Volume (ft^3):	6,975				
Diameter (ft)	13.6				
Residence time per tank (hrs):	4				
Catalyst:	Immobilized *R. rhodochrous J1* biocatalyst in polyacrylamide gels				
Utilities:					
Refrigeration (ton/day):	30,876				
Comments: Three stirred tank reactors in series.					
*Cost per tank, includes 2 impellers (turbines)					

Feed Storage Tank

Identification:	Item:	*Floating Roof Storage Tank*				
	Item No.:	*T-101*			Date:	*4/10/13*
	No. Required:	*1*			By:	*JS/AC/PB/AL*
	C_p ($):	*206,429*			C_{BM} ($):	*629,609*

Function: MPDA feed storage tank.

Operation: Continuous

	S-101 Outlet				
Materials Handled:					
Total Flow (lb/hr):	3,307				
Volumetric Flow (ft^3/hr):	54				
Component Flows (lb/hr):					
O_2	0				
H_2	0				
N_2	0				
Ammonia	0				
H_2O	0				
CO_2	0				
MPDA	3,307				
3-methylpiperidine	0				
3-picoline	0				
3-cyanopyridine	0				
Niacinamide	0				
Temperature (°F):	77				
Pressure (psi):	14.5				
Vapor Fraction:	0				

Design Data:

V (gallons):	77,000
τ (hr):	168.0
Type:	Floating Roof
Material:	Stainless Steel

Utilities:

Comments:

Product Storage Tank

Identification:	Item:	*Cone-roof storage tank*			
	Item No.:	*T-301*		Date:	*4/10/13*
	No. Required:	*1*		By:	*JS/AC/PB/AL*
	C_p (\$):	*104,337*		C_{BM} (\$):	*434,044*

Function: Niacinamide product storage tank.

Operation: Continuous

	S-316 Inlet				
Materials Handled:					
Total Flow (lb/hr):	3,453				
Volumetric Flow (ft^3/hr):	44				
Component Flows (lb/hr):					
O_2	0				
H_2	0				
N_2	0				
Ammonia	0				
H_2O	0				
CO_2	0.2				
MPDA	Trace				
3-methylpiperidine	28				
3-picoline	24				
3-cyanopyridine	29				
Niacinamide	3,372				
Temperature (°F):	77				
Pressure (psi):	14.5				
Vapor Fraction:	0				

Design Data:

V (gallons):	93,000
τ (hr):	168
Type:	Cone-Roof
Material:	Carbon Steel

Utilities:

Comments:

E. Equipment Cost Summary

The table below outlines all of the bare-module costs for the equipment used in this process. A majority of the purchase costs were found using ASPEN IPE, which used 2010 cost indices. The cost was updated to reflect 2013 cost indices before being added into the table. For most of the heat exchangers, compressors, blowers, neutralizer, and storage tanks, correlations present in *Product and Process Design Principles* were used to find the cost of the vessel. Purchase costs were then converted from the 2006 values (CE=500) to 2013 values (CE=570). Sample calculations can be found in Appendix IX. The cost of the reactors and the decolorizing unit were found using correlations associated with the vessel size and standard equipment that closely modeled the units. To find the total cost of the equipment, the purchase cost was multiplied by the bare module factor. Equipment unit numbers marked with an asterisk indicate that the bare module cost is a combination of equipment with different bare module factors, and hence does not follow the purchase cost multiplied by bare-module factor formula. The bare-module factor, which includes allowances for cost of installation materials, installation labor, freight, taxes, insurance, construction overhead, and contractor engineering expenses, is specific to each type of equipment and may be found in Table 22.11 of *Product and Process Design Principles*. Total bare module cost for all of the equipment pieces is $34 million, which includes the cost for spare pumps for the process.

Table E1. Equipment Cost Summary

Equipment Cost Summary					
Unit #	**Equipment Type**	**Costing Method**	**Purchase Cost**	**F_{BM}**	**C_{BM}**
A-101	Absorber	IPE	791,116	4.16	3,291,044
A-102	Absorber	IPE	548,989	4.16	2,283,795
B-201	Blower	Seider	2,555	2.15	5,492
B-202	Blower	Seider	2,304	2.15	4,954
B-203	Blower	Seider	2,828	2.15	6,080
C-101	Compressor	Seider	40,335	2.15	86,719
C-102	Compressor	Seider	94,138	2.15	202,397
C-103	Compressor	Seider	118,025	2.15	253,753
C-301	Compressor	Seider	1,084,345	2.15	2,331,342

Equipment Cost Summary (*continued 1*)					
Unit #	**Equipment Type**	**Costing Method**	**Purchase Cost**	**F_{BM}**	**C_{BM}**
D-101	Distillation Column	IPE/Seider	967,255	4.16	4,023,779
DC-301*	Decolorizing Unit	Correlations	38,089	4.16	149,787
DR-301	Dryer	Vendor	804,369	2.06	1,657,000
F-201	Flash Vessel	IPE	128,760	4.16	535,640
F-301	Flash Vessel	IPE	115,273	4.16	479,535
HX-101	Heat Exchanger	IPE	76,656	3.17	243,001
HX-102	Heat Exchanger	IPE	74,697	3.17	236,789
HX-201	Heat Exchanger	IPE	133,947	3.17	424,612
HX-202A	Heat Exchanger	IPE	104,322	3.17	330,700
HX-202B	Heat Exchanger	IPE	77,117	3.17	244,462
HX-203	Heat Exchanger	IPE	57,636	3.17	182,707
HX-204	Heat Exchanger	IPE	57,636	3.17	182,707
HX-205	Heat Exchanger	IPE	72,622	3.17	230,211
HX-206	Heat Exchanger	IPE	53,371	3.17	169,187
HX-301	Heat Exchanger	IPE	66,282	3.17	210,113
HX-302	Heat Exchanger	IPE	123,457	3.17	391,359
HX-303	Heat Exchanger	IPE	56,829	3.17	180,149
HX-304A	Heat Exchanger	IPE	253,139	3.17	802,450
HX-304B	Heat Exchanger	IPE	88,414	3.17	280,273
N-301*	Neutralizer	Seider	45,900	4.16	142,736
P-101	Pump	Seider	30,547	3.30	100,806
P-102	Pump	Seider	30,432	3.30	100,426
P-103	Pump	Seider	41,844	3.30	138,085
P-201	Pump	Seider	34,467	3.30	113,740
P-202	Pump	Seider	34,467	3.30	113,740
P-203	Pump	Seider	34,467	3.30	113,740
P-204	Pump	Seider	31,239	3.30	103,088
P-301	Pump	Seider	36,541	3.30	120,587
R-101	Tubular Reactor	Correlations	810,184	3.17	2,568,283
R-102	Packed Bed Reactor	Correlations	30,713	3.17	97,359
R-201	Tubular Reactor	Correlations	721,219	3.17	2,286,265
R-202A*	Semi-continuous stirred tank reactor	Correlations	268,719	3.17	918,160
R-202B*	Semi-continuous stirred tank reactor	Correlations	268,719	3.17	918,160
R-202C*	Semi-continuous stirred tank reactor	Correlations	268,719	3.17	918,160
T-101	Storage Tank	Seider	206,429	3.05	629,609
T-301	Storage Tank	Seider	104,337	4.16	434,044
PS-101	Spare Pump	IPE	30,547	3.30	100,806
PS-102	Spare Pump	IPE	30,432	3.30	100,426

Equipment Cost Summary (*continued 2*)					
Unit #	**Equipment Type**	**Costing Method**	**Purchase Cost**	**F_{BM}**	**C_{BM}**
PS-103	Spare Pump	IPE	41,844	3.30	138,085
PS-201	Spare Pump	IPE	34,467	3.30	113,740
PS-202	Spare Pump	IPE	34,467	3.30	113,740
PS-203	Spare Pump	IPE	34,467	3.30	113,740
PS-204	Spare Pump	IPE	31,239	3.30	103,088
PS-301	Spare Pump	IPE	36,541	3.30	120,587
		Total Bare-Module Cost		**$**	**33,769,035**

F. FIXED-CAPITAL INVESTMENT SUMMARY

The fixed costs for the plant stem from mostly the equipment costs, previously reported by unit in the equipment costs summary in Section E: Table E1. Other factors that influence that total permanent investment are summarized in Table F1. The fixed capital investment, summarized in Table F2, details the capital investment required for the entire process. The direct permanent investment, C_{DPI} is the sum of the total bare-module equipment costs, the site preparation costs, the service facilities costs and allocated costs. From table E1, the total Bare-Module Cost is $33,700,000, which includes the cost of storage tanks and process machinery and the spare pumps for the process.

Table F1. Summary of Total Permanent Investment, TPI factors

Cost of Site Preparations:	5%	of Total Bare Module Costs
Cost of Service Facilities:	5%	of Total Bare Module Costs
Allocated Costs for utility plants and related facilities:	$500,000	
Cost of Contingencies and Contractor Fees:	18%	of Direct Permanent Investment
Cost of Land:	2%	of Total Depreciable Capital
Cost of Royalties:	2%	of Total Depreciable Capital
Cost of Plant Start-Up:	10%	of Total Depreciable Capital

The costs of site preparation and service facilities are estimated to be 5.00% of the total bare-module cost as recommended in *Product and Process Design Principles*. This estimate is considered conservative for most plant setups and locations. While some utilities are readily available onsite (for example the cooling water, steam, hot water) others like Dowtherm heating system and the refrigeration system are not; thus the allocated costs of $500,000 for utility plants and related facilities for the two heating and refrigeration systems will be set aside. As previously mentioned, the Dowtherm system was priced at around $700,000. However, the two refrigeration systems that will need to be put into the plant will be less expensive than this Dowtherm system. Therefore a rough estimate of $500,000 is used to cover the cost of these refrigeration units.

The cost of contingencies and contractor fees, accounted for in the total depreciable capital, C_{TDC}, at 18%, is a combination of a 15% allowance for direct permanent investment (DPI) for contingencies and a 3% allowance for contractor fees. Contingencies are estimated at 15% of the DPI because the technologies throughout the process are readily available, except for the biocatalyst present in the fourth reactor. 15% of the DPI allocated to contingencies is reasonable to cover any expenses associated with unplanned events. Allocating 2% of the TDC toward land is reasonable since this plant and the equipment is relatively available and should not have issues securing land in regions close to MPDA production for the feedstock. Additionally, 2% of the TDC is allocated to royalties, as recommended in *Product and Process Design Principles* because this process is based on a patent currently owned by Lonza. As for the startup costs, 10% is used because fuel for the Dowtherm is required as well as startup capital needed for MPDA storage at the plant.

Listed below is the overall fixed capital investment summary, taking into account the above considerations. Table F2 outlines the total permanent investment.

Table F2. Summary of Fixed Capital Investment

Investment Summary				
Bare Module Costs				
Fabricated Equipment	$	16,672,036		
Process Machinery	$	3,794,948		
Spares	$	904,211		
Storage	$	1,063,653		
Other Equipment	$	8,747,659		
Catalysts	$	2,586,528		
Computers, Software, Etc.	$	-		
Total Bare Module Costs:			**$**	**33,769,035**
Direct Permanent Investment				
Cost of Site Preparations:	$	1,688,452		
Cost of Service Facilities:	$	1,688,452		
Allocated Costs for utility plants and related facilities:	$	500,000		
Direct Permanent Investment			**$**	**37,645,938**
Total Depreciable Capital				
Cost of Contingencies & Contractor Fees	$	6,776,269		
Total Depreciable Capital			**$**	**44,422,207**
Total Permanent Investment				
Cost of Land:	$	888,444		
Cost of Royalties:	$	0		
Cost of Plant Start-Up:	$	4,442,221		
Total Permanent Investment - Unadjusted			$	49,752,872
Site Factor				1.00
Total Permanent Investment			**$**	**49,752,872**

G. OTHER IMPORTANT CONSIDERATIONS

Environmental and Safety Considerations

Given the nature of the project, environmental considerations are important to the overall sustainability of this process. Waste treatments and chemical leakage are two leading concerns. The waste products include CO_2, a small amount of NOx, as well as the organic compounds left in the purge stream after leaving the dryer. The first two will be rectified using wet scrubbers at the exits of the streams. Additionally, although the amount of CO_2 produced by the biocatalysts was not determined due to insufficient data, wet scrubbers will be placed at the vents of each CSTR. Regeneration of the catalysts also produces CO_2, which will be redirected to one of the wet scrubber units. Finally, the organic compounds in the wastewater will be treated at an off-site facility.

The environmental impact of a chemical process can be quantified via the Waste Reduction (WAR) algorithm, made available by the U.S. Environmental Protection Agency (USEPA). The WAR algorithm utilizes life cycle analysis and investigates areas such as human toxicity, ozone depletion, global warming and terrestrial toxicity potentionals when calculating the overall potential environmental impact (PEI). The lower the PEI, the less impact the process has on the environment. The total rate of PEI leaving a system per hour is defined as I_{out} (Fermeglia et al, 2007). Using the WAR software downloaded from the EPA website, the authors attempted a preliminary environmental assessment to evaluate the I_{out}. I_{out} for the production of niacinamide was calculated to be 35 PEI/hr. When compared to other PEI values, all within the range of 35 to 160 PEI/hr, this process rates well, validating its overall sustainability (Fermeglia et al, 2007; Gangadharan et al, 2012; Seay and Gish, 2010).

The high-pressure hydrogen system designed to vaporize the Dowtherm A is another point of caution. Given its high flammability potential upon leaking, extra care must be exercised when performing leak tests on this part of the process. In addition, leaks can be guarded against via welded joints and shut-off valves periodically placed within the piping.

The two most toxic chemicals in our process are Dowtherm A and ammonia. In both cases, stringent leak and purge tests will be performed prior to starting production. Moreover, control equipment including valves, feedback loops, and computer regulation will be used to monitor the Dowtherm A and ammonia content in the air surrounding relevant vessels and piping, to ensure safe working conditions for operators.

Dust explosions and fires are a potential hazard with regard to the handling of niacinamide in powder form. Larger particles (greater than 50 μm) are desired to reduce the risk of explosions, as higher surface areas result in greater exposure to heat and oxygen and thus greater potential to ignite. To best assess the risk of explosion, the volume (electrical) resistivity of the powder should be measured. The lower the resistivity, the lower the risk of explosion (Lonza Plant Safety, 2012).

Finally, transient operating conditions during startup and shutdowns may lead to undesirable and unsafe changes in process variables such as temperature and pressure, especially with regard to the Dowtherm A furnace and the exothermic tubular reactors. After startup, there is still the concern of high temperatures and possibly high pressures, but the safety issues associated with these are usually much less. To avoid issues such as thermal runaway, the process and controls will be closely monitored during startup and shutdown. Detailed process safety management plans will be disseminated throughout the plant for each process unit. Pressure and temperature controls as well as pressure-relief valves will be located throughout the process, including vaporizers and heat exchangers with large temperature changes.

A quantitative analysis of the safety of the process and its chemicals may be performed using one of several methods, including the Dow Fire and Explosion Hazard Index, Hazard and Operability Analysis (HAZOP), and the Prototype Index of Inherent Safety (PIIS) (Gangadharan et al, 2012).

Necessary personal protective equipment such as gloves, goggles, lab coats, face-masks and close-toe shoes will be required to prevent harm from contact with any of the organic compounds in the process, as most are corrosive and toxic if skin-contacted or inhaled. Please refer to the MSDS sheets in Appendix IX for further information.

Catalyst Regeneration

Catalysts eventually become deactivated via various methods, the most common being carbon deposits (coking), sintering and poisoning. Coking is the main concern within this process. There are two main options for handling deactivated catalysts: discarding the catalyst completely and purchasing new catalyst each cycle, and regenerating the catalyst on-site every cycle. There are two further options associated with the latter. First, an extra reactor may be purchased to allow for continuous operation; while one reactor is being regenerated, the other remains running. Second, more commonly, the plant may be shut down as necessary to regenerate the catalyst periodically.

To remain sustainable in this process, whenever possible it is desirable to regenerate the catalysts. Due to the low concentration of hydrocarbons in the process, the catalysts in the first and third reactors only require regeneration every six months, entailing on-site regeneration in the form of taking each reactor off-line and combusting off the coke. It was deemed too costly to buy an entire duplicate reactor solely for regeneration purposes. The entire regeneration process is estimated to take one day. Oxygen will be pumped through the reactor and combusted with the carbon, following the simple reaction:

$$C + O_2 \rightarrow CO_2 \tag{7}$$

Due to limited information from the patents, other literature references were sought to determine the required flow of oxygen assuming that carbon would account for 3% of the catalyst's original mass (Trimm, 2001). Oxygen flow rates of 448 lbs/6 months and 21,048 lbs/6 month were calculated for the first and third reactors, respectively.

Since the third reactor contains the precious metal Palladium, Pd, and also has an activation life of at least one year according to the Lonza patent, it will be removed and replaced with new catalyst once every year, again requiring a one day shutdown. However, according to one of our industrial consultants, Mr. Kolesar, we will be able to recover roughly 70% of the catalysts cost. Considering the Pd-SiO_2/Al_2O_3 costs $783,000 to purchase, we will be able to recover $548,000 each year, yielding a net cost of $235,000 .

Finally, due to the nature of biocatalysts, once they have died they must be discarded and new ones purchased. We will renew the biocatalysts in reactor four once per year. All regenerations will be performed in conjunction with required safety and maintenance plant shutdowns to reduce the amount of off-line time for the plant. Refer to page 234 for Sample Calculations for catalyst regeneration.

Startup Considerations

There are several key issues to consider during start up. First, an inert gas must be run through the process to test for leaks. Controlled process variables such as temperature, pressure, inventory (material level in storage tanks), material composition, and flow are often not at their steady-state value during startup – extra caution must be exercised. Operation conditions may also need to be adjusted initially; for example, the exothermic tubular reactors may need to run at higher initial temperatures to yield the same conversion to obtain the appropriate product quality. Furthermore, bypass pipes may be needed until the desired steam compositions are reached for proper produce quality. Finally, units such as the distillation tower and flash vaporizers may initially need water or steam injected in until the correct operating conditions are reached. (Verwijs, 1995). Many of these considerations can be furthered specified after a pilot plant has been constructed.

For the plant to run properly during initial startup as well as after any stop in niacin production for necessary maintenance or catalyst regeneration, the furnace for the Dowtherm system must have a feed stock other than the hydrogen produced in the process. To keep with the overarching theme of environmental cleanliness, the feed stock chosen will reduce emissions of “green-house” gases such as carbon monoxide and carbon dioxide. Natural gas, the conventional fuel of choice, was not chosen for this startup process due to its negative effects on the environment. The startup fuel chosen is renewable natural gas, a type of biogas upgraded to natural gas quality (BioSNG, 2007). Biogas is captured from the decomposition of organic material in places such as landfills, sewage treatment facilities, and farms (animal byproducts). Impurities such as carbon dioxide, water, and hydrogen sulfide are then removed from the raw biogas. Once upgraded, biogas may be substituted directly for natural gas (Alternative Fuels

Data Center, 2013). The cost for renewable natural gas is around \$9.75-\$11/MMBtu, adjusted for 2013 prices (Rutledge, 2005). Though this up-production makes renewable natural gas more expensive than traditional natural gas, the environmental benefits further enhance the green nature of our process.

Additionally, we will be shipping our supply of MPDA from Invista, a company located nearby the plant in Ontario. Given the volume we will require for storage, ISO containers will be used during shipping (Invista, 3).

Finally, upon process startup, there will be a minimum delay of at least 12 hours to account for the four-hour residence times for each CSTR.

Purity Improvement

To improve the purity of the niacinamide¸ a similar separation scheme utilized by Lonza’s plant in Guangzhou, China could be used, in which a toluene extraction unit is placed after the third reactor to retain and extract the 3-cyanopyridine that is produced in that reaction (ICIS.com, 1999). In doing so, the remainder of the materials are recycled back into the third reactor. This not only simplifies the separation later on in the synthesis, but also increases the rate of conversion of the previous products into 3-cyanopyridine. This solution may then be distilled yielding a pure 3-cyanopyridine product and toluene, which can be recycled back into the extraction column. The timeline for this project did not allow for the investigation of this particular purification step; however, if this separation scheme were pursued further, not only would it increase the conversion of the other intermediates, but it would also increase the purity of the niacinamide after the final drying process, as there will be less organic compound impurities present in the niacinamide powder mixture. Although toluene is a toxic organic molecule that would make the process less green, it would operate in a closed loop such that only trace amounts of toluene would escape, limiting the waste released.

Schedule

The plant is expected to operate 335 days per year, allowing 30 days of down time. The process must be shut down periodically to allow for safety inspections, maintenance, catalyst regeneration, and CSTR cleaning. The CSTRs must be taken off-line and given steam-in-place (SIP) treatments as well as clean-in-place (CIP) treatments, which can be completed within one working day. To minimize the amount of off-line time, the catalyst regeneration and cleaning of the CSTRs will occur simultaneously (Wildy, 2003).

Miscellaneous

To best prepare for issues outside of our control, several contingency plans will be implemented. Firstly, bypass lines will be built into the CSTR reactor set in the case that one reactor fails. Residence times will be adjusted accordingly. Secondly, pressure and temperature controls will dictate the maximum pressures and temperature differences allowed before safety systems are implemented. Once the process plant is built, it will be easier to identify possible problem areas and adjust accordingly.

Due to the slurry mixtures involved in our process streams, it should be noted that to prevent clogs and pump failure, it is necessary to fit the pipes with filters. If further research into this process is desired, it is recommended that filters be included in the pressure drop calculations for equipment specifications. Solids complicate the flow within a process, and there must always be enough liquid to ensure proper flow through pipes and vessels. Accordingly, spare pumps (one for each size) will be stored onsite in the case of equipment failure.

Lastly, it was proposed that the excess hydrogen in our process be used to power a fuel cell to generate electricity rather than fuel the Dowtherm system. However, the 2.5% impurities within the hydrogen stream are too high for a fuel cell membrane to function properly and efficiently. Although it would have increased the sustainability of our project, in the end it was not feasible.

H. ENERGY BALANCE AND UTILITY REQUIREMENTS

Energy Balance

This section illustrates the energy balance and necessary utility requirements of the niacinamide production plant. However, this section does not include a detailed description of the energy consumption or utility requirements of the dryer due to limited data. For this unit, a rough estimate has been made based on data found on other similar spray drying processes. In addition, the energy balance and utility requirements of the decolorizer and neutralizer in the process were not calculated and have been assumed to be negligible in the overall process. This production plant as a whole requires a 20 MMBTU/hr addition with a net electricity requirement of 2,321 HP. The unit number, equipment type, energy requirements, and possible methods to satisfy the energy requirement of the equipment are listed in the table below. The units are grouped according to number and method used to satisfy the energy requirements.

Table H1. Utility descriptions based on unit number.

Unit #	Equipment Type	Energy Requirement	Methods to Satisfy Energy Requirement
B-201	Blower	2.3 HP	Electricity
B-202	Blower	2.0 HP	Electricity
B-203	Blower	2.6 HP	Electricity
C-101	Compressor	22.3 HP	Electricity
C-102	Compressor	73.7 HP	Electricity
C-103	Compressor	101.3 HP	Electricity
C-301	Compressor	2,112.3 HP	Electricity
P-101	Pump	0.4 HP	Electricity
P-102	Pump	0.005 HP	Electricity
P-103	Pump	0.7 HP	Electricity
P-201	Pump	0.3 HP	Electricity
P-202	Pump	0.3 HP	Electricity
P-203	Pump	0.6 HP	Electricity
P-204	Pump	0.6 HP	Electricity
P-301	Pump	1.7 HP	Electricity
A-102	Dowtherm Process	-8 MMBTU/hr	Hydrogen Fuel
D-101	Condenser	-6.9 MMBTU/hr	Cooling Water
HX-202A	Heat Exchanger	-4.4 MMBTU/hr	Cooling Water
HX-304A	Heat Exchanger	-33 MMBTU/hr	Cooling Water
R-101	Reactor	-0.45 MMBTU/hr	Cooling Water
R-201	Reactor	-5.9 MMBTU/hr	Cooling Water
A-101	Condenser	-2.8 MMBTU/hr	Suva Refrigeration
A-102	Condenser	-1.2 MMBTU/hr	Ethylene Refrigeration
HX-202B	Heat Exchanger	-0.95 MMBTU/hr	Suva Refrigeration
HX-203	Heat Exchanger	-0.007 MMBTU/hr	Suva Refrigeration
HX-204	Heat Exchanger	-0.006 MMBTU/hr	Suva Refrigeration
HX-205	Heat Exchanger	-0.19 MMBTU/hr	Suva Refrigeration
HX-304B	Heat Exchanger	-1.7 MMBTU/hr	Suva Refrigeration
R-202A	CSTR in Series Reactor	-1.1 MMBTU/hr	Suva Refrigeration
HX-206	Heat Exchanger	0.22 MMBTU/hr	Hot Water
HX-301	Heat Exchanger	1.2 MMBTU/hr	Hot Water
A-101	Reboiler	1.7 MMBTU/hr	Steam
A-102	Reboiler	0.82 MMBTU/hr	Steam
D-101	Reboiler	6.4 MMBTU/hr	Steam
HX-302	Heat Exchanger	29 MMBTU/hr	Steam
HX-303	Heat Exchanger	0.002 MMBTU/hr	Steam
HX-101	Heat Exchanger	1.5 MMBTU/hr	Dowtherm
HX-102	Heat Exchanger	0.29 MMBTU/hr	Dowtherm
HX-201	Heat Exchanger	2.6 MMBTU/hr	Dowtherm
R-102	Packed Bed Reactor	2.6 MMBTU/hr	Dowtherm

Utility Requirements

In an attempt to reduce cost and increase plant efficiency, the utility requirements were integrated as much as possible throughout the process. By integrating available heat from the Dowtherm cycle into the heat exchangers and reactors that need a net input of heat, the utilities necessary from outside of the plant decrease significantly. The 8 MMBTU/hr available by burning the hydrogen created in the process can be used to heat the Dowtherm cycle and in turn be distributed to multiple heat exchangers and R-102 for heating. Since data was not available on the decolorizer and the neutralizer, and these vessels operate at room temperature and atmospheric pressure, these units have been again left out of the utility requirement calculations.

Utilities are calculated based on the assumption that they can be purchased directly from utility companies in the plant region. Prices are estimated using Table 23.1 of Product and Process Design Principles with adjusted prices from 2006 (CE=500) to 2013 (CE=570). The prices were adjusted from the table accordingly. Outlined below are short descriptions of each utility required followed by tables illustrating the required energy according to units.

Electricity

The overall process requires 2,321 HP to pumps and compressors. Electricity is assumed to be available at a price of $0.068/kW-hr, adjusted for 2013. The infrastructure associated with electricity totals to around $942,900, or around 19% of the total cost for utilities.

Cooling Water

Cooling water is assumed to be used at an inlet pressure of 65 psi and inlet temperature of 90°F with an exit temperature of 120°F. This process requires 1,690,000 lb/hr of cooling water in total. This water is available for $0.0855/1,000 lb, as adjusted to reflect prices for 2013. 120°F reflects the maximum outlet temperature allowed for cooling water without further processing necessary. To work in the heat exchangers, a minimum temperature difference of 10° is used. Cooling water will cost $1,159,000 in utilities, accounting for 23% of the total cost.

Dowtherm

Hydrogen created during the process will be separated out and account for the fuel necessary to heat the Dowtherm process. 8 MMBTU/hr is generated assuming a 99% conversion of the hydrogen. This heat will be transferred to the heat exchangers HX-101, HX-102, and HX-201 and reactor R-102. Dowtherm A was chosen for this process, which is a eutectic mixture of biphenyl and diphenyl oxide. An MSDS report for this chemical is presented in Appendix IX. The cost of this process is included as a whole in the utilities. Sample calculations for this system are present in the Appendix IX page 240.

Refrigeration

The coolant used for the refrigeration in the process was -15 °F cooling fluid. R-134a, also know from DuPont as Sura-134a, is used as the refrigerant due to its temperature range for the process, at the lowest temperature, -15 °F. This is the closest available refrigerant that meets the needs of process cooling. In accordance with green principles, this refrigerant does not propagate a flame under normal conditions and also shows no evidence of toxicity below 400 ppm, while also not depleting the ozone layer. For these calculations, the overall cost of refrigeration also includes the electricity needed to pump and cool the refrigerant. Appendix IX outlines the chart used to calculate the needed amount , per ton, of refrigeration.

The MSDS for Sura-134a is given in Appendix IX. The refrigeration process used for A-102 at the condenser, however, needs to be at a lower temperature to achieve the desired separation. Ethylene is chosen for this process due to its low temperature range of -100 to -150°F; the condenser needs to be cooled from 90°F to a temperature of -117°F. Overall the process requires 220,800 ton-day of refrigeration. Both ethylene and R-134a are assumed to be taken from offsite refrigeration systems; the cost of these systems is incorporated into the overall cost per lb of the refrigerants. To refrigerate, the cost of cooling is $2.44 per ton-day for R-134a whereas the cost for ethylene refrigeration is $3.99 per ton-day. The total cost for refrigeration is $590,900, which is approximately 12% of the total utility cost. Please refer to page 239 for Refrigeration Power Requirements chart to calculate energy requirements.

Hot Water

For two of the heat exchangers in the process, streams need to be heated to well below the operation temperatures of steam. Therefore, two streams for HX-206 and HX-301 of hot water are used as utilities, at 100F. This hot water accounts for 1,453,000 BTU/hr at a cost of $0.855 per lb, scaled to 2013 costing. This totals the annual cost to $8,300, which is around 0.2% of the total cost for utilities.

Steam

The steam selected for the heating of HX-108 and the reboiler of D-101 is used to vaporize the streams and increase the temperature. High pressure steam had to be used, with a saturation temperature of 450 psig steam at 460°F, which is higher than any of the stream temperatures that use steam for heating. The heating value is assumed to be 1205 BTU/lb steam. The cost for steam is around $7.52/1,000 lbs, which would total to $1,900,000, or about 39% of the total utility costs. This accounts for the largest cost contribution for utilities in this process.

Wastewater

The wastewater streams generated in this process include mostly ammonia as contaminants. Because ammonia is listed as a toxin in water, the EPA has strict standards and regulations on what concentration ammonia is able to be released from chemical plants (Srinivasan et al., 2008). A packed bed air stripping unit must be added to remove the ammonia present in the wastewater stream. Therefore, costs were not calculated based on the weight of contaminant but instead based on the operating costs of an air stripping unit for the wastewater stream (Stocking, et al, 2000). In this unit, air is fed in large excess to remove ammonia from the water and usually adsorb into the packing material of the stripping unit (Lantec, 2004 and Huang & Shang, 2006). EPA regulations specify that wastewater can have a maximum of 0.14 mg ammonia/L (200 ppm) (EPA Emergency Management, 2004). The overall cost is $239,065 for the first year to remove ammonia from the wastewater stream S-319. In subsequent years, the cost of this unit will only be upkeep. This is around 5% of the total cost of utilities.

Waste Gas

Two streams may require treatment in the process. S-314 is the nitrogen purge from the nitrogen recycle stream. However, EPA regulations allow between 2 and 10 PPM ammonia as slip levels (US EPA, 2001 and Phillips, 1995). In this process, ammonia appears as 87 PPM in the nitrogen purge stream. The only other components present are oxygen, water vapor, and small amount of hydrogen. Therefore this stream requires further processing before it can be vented to the atmosphere. The other stream, S-115, which would later result in the byproduct of burning hydrogen for the Dowtherm heating cycle, ammonia is theoretically in upwards of 35 PPM with carbon dioxide at 914 PPM. Depending on the operating conditions and the flow rate of the excess air in the process, NOx will also form in the process since air is added to burn the hydrogen feed. Although there are no regulations on carbon dioxide, ammonia and NOx byproducts must be removed from the stream. The best choice to clean both of these streams is a wet scrubber (Phillips, 1995 and Ohio EPA, 1993) which effectively removes NOx and ammonia from the waste gas stream. The overall cost of $80,000 is outlined in the table and is based on the cost of operation to remove NOx, ammonia, and pretreating costs before the streams can be introduced into the wet scrubber. These two units account for around 2% of the utility cost.

Table H2. Utility usage and costs by utility type.

Electricity				
Unit #	**Usage (kW)**	**Duty (HP)**	**Cost ($/hr)**	**Annual Cost ($)**
B-201	1.7	2.3	0.12	938
B-202	1.5	2.0	0.10	819
B-203	2.0	2.6	0.13	1,071
C-101	16.5	22.3	1.13	9,068
C-102	54.6	73.7	3.73	29,952
C-103	75.0	101.3	5.13	41,153
C-301	1,563.1	2,112.3	106.92	858,109
P-101	0.3	0.4	0.02	156
P-102	0.003	0.005	0.000	2
P-103	0.5	0.7	0.04	302
P-201	0.2	0.3	0.01	120
P-202	0.2	0.3	0.01	114
P-203	0.4	0.6	0.03	229
P-204	0.4	0.6	0.03	224
P-301	1.2	1.7	0.08	671
Total	**1,718**	**2,321**	**117.48**	**942,929**

Cooling Water				
Unit #	**Usage (lb/hr)**	**Duty (BTU/hr)**	**Cost ($/hr)**	**Annual Cost ($)**
D-101	231,886	-6,933,102	19.83	159,125
HX-202A	146,388	-4,376,827	12.52	100,455
HX-304A	1,099,120	-32,862,379	93.97	754,242
R-101	15,118	-452,000	1.29	10,374
R-201	196,694	-5,880,900	16.82	134,976
Total	**1,689,205**	**-50,505,208**	**144.43**	**1,159,171**

Dowtherm A		
Unit #	**Duty (MMBTU/hr)**	**Annual Cost ($)**
HX-101	1.468	--
HX-102	0.293	--
HX-201	2.600	--
R-102	2.602	--
Total	**6.963**	**722,207**

Refrigeration				
Unit #	**Usage (ton-day)**	**Duty (BTU/hr)**	**Cost ($/ton-day)**	**Annual Cost ($)**
A-101	76,943	-2,810,700	2.44	187,710
A-102	33,598	-1,227,340	3.99	134,058
HX-202B	26,057	-951,843	2.44	63,568
HX-203	199	-7,284	2.44	486
HX-204	178	-6,495	2.44	434
HX-205	5,064	-185,000	2.44	12,355
HX-304B	47,967	-1,752,230	2.44	117,021
R-202A	30,876	-1,127,900	2.44	75,326
Total	**220,883**	**-8,068,792**	**2.44**	**590,958**

Hot Water (100 F)				
Unit #	**Usage (lb/hr)**	**Duty (BTU/hr)**	**Cost ($/hr)**	**Annual Cost ($)**
HX-206	185	223,000	0.16	1,270
HX-301	1,021	1,230,000	0.87	7,005
Total	**1,206**	**1,453,000**	**1.03**	**8,275**

Steam (450 psi)				
Unit #	**Usage (lb/hr)**	**Duty (BTU/hr)**	**Cost ($/hr)**	**Annual Cost ($)**
A-101	1,401	1,687,610	10.54	84,573
A-102	682	821,359	5.13	41,162
D-101	5,304	6,391,715	39.91	320,316
HX-302	24,002	28,922,000	180.59	1,449,403
HX-303	2	2,431	0.02	122
Total	**31,390**	**37,825,115**	**236.18**	**1,895,576**

Wastewater Treatment			
Stream	**Unit Cost ($)**	**Cost ($/year)**	**Annual Cost ($)**
S-319	125,000	114,065	239,065
Total	**125,000**	**114,065**	**239,065**

Wastegas Treatment			
Stream	**Unit Cost ($)**	**Cost ($/year)**	**Annual Cost ($)**
S-314	35,000	5,000	40,000
S-115	35,000	5,000	40,000
Total	**70,000**	**10,000**	**80,000**

Total Utilities	**$4,911,573**
Dowtherm System	**$722,207**

I. Operating Cost and Economic Analysis

The economic analysis is based on results calculated using the Profitability Analysis Spreadsheet 3.0 provided by *Seider et al., 2009.* Table I.1 is a summary of an operating time-table and assumptions that are used to perform the analysis. An overall inflation rate of 2% is assumed.

Table I.1. Summary of Economic Analysis Inputs

General Information					
Process Title:	**Green Process to Produce Niacin**				
Product:	**Niacinamide**				
Plant Site Location:	**Michigan**				
Site Factor:	**1.00**				
Operating Hours per Year:	**8026**				
Operating Days Per Year:	**334**				
Operating Factor:	**0.9162**				
Product Information					
This Process will Yield					
		3,452 lb of Niacinamide per hour			
		82,836 lb of Niacinamide per day			
		27,701,739 lb of Niacinamide per year			
Price		**$4.43 /lb**			
Chronology					
Year	**Action**	**Distribution of Permanent Investment**	**Production Capacity**	**Depreciation** 5 year MACRS	**Product Price**
2013	Design		0.0%		
2014	Construction	100%	0.0%		
2015	Production	0%	45.0%	20.00%	$4.43
2016	Production	0%	67.5%	32.00%	$4.52
2017	Production	0%	90.0%	19.20%	$4.61
2018	Production		90.0%	11.52%	$4.70
2019	Production		90.0%	11.52%	$4.80
2020	Production		90.0%	5.76%	$4.89
2021	Production		90.0%		$4.99
2022	Production		90.0%		$5.09
2023	Production		90.0%		$5.19
2024	Production		90.0%		$5.30
2025	Production		90.0%		$5.40
2026	Production		90.0%		$5.51
2027	Production		90.0%		$5.62
2028	Production		90.0%		$5.73
2029	Production		90.0%		$5.85
2030	Production		90.0%		$5.96
2031	Production		90.0%		$6.08
2032	Production		90.0%		$6.21

Operating Cost Summary

Variable Costs

Variable costs for the plant include raw materials, utilities, and other expenses. The variable cost does not include revenue from selling value-added byproducts since this process does not generate them. Other expenses include, but are not limited to, management incentives, administrative expenses, research and laboratory costs, and sales and marketing expenses. Also, since this process is based off a patent by Lonza, research must be done to improve the process and equipment. Direct research is then estimated at 4.8% of the sales cost and allocated research at 0.5%.

MPDA is the primary raw material used in this process. Oxygen, nitrogen, and process water, which was also priced on a basis of one pound of niacinamide produced, are other necessary raw materials. MPDA is around $3.09 per pound, or $31 per tonne of liquid raw material. This price has included pipeline costs and any other transportation fees that may be associated with the MPDA. For each pound of niacinamide produced, 0.96 pounds of MPDA are required. As for oxygen and nitrogen, these will be brought to the plant on trailers which contain 20 MT. Assuming a cost of $200 per megaton with a 10% variable on the costing, which would include the storage tank, pump, and ambient vaporizer, 0.43 pounds of oxygen per pound of niacinamide is needed. The same process is true for nitrogen; this would come to the plant for $70/MT plus 10% variable cost. For every pound of product produced, 0.0090 pounds of nitrogen is needed. As for process water, 0.35 pounds of water are necessary for every pound of product. The process water comes at a cost of $0.75 per pound.

Utilities are another concern in terms of the variable cost. This were discussed in a previous section titled Utilities and Energy Balances. All utility costs have been obtained from Product and Process Design Principles as mentioned below. Outlined in Table I.2 below is the total variable cost of the process.

Table I.2. Summary of Variable Cost

Variable Cost Summary			
Variable Costs at 100% Capacity:			
General Expenses			
Selling / Transfer Expenses:		$	3,683,072
Direct Research:		$	5,892,915
Allocated Research:		$	613,845
Administrative Expense:		$	2,455,381
Management Incentive Compensation:		$	1,534,613
Total General Expenses		$	14,179,828
Raw Materials	$2.96 per lb of Niacinamide		$82,042,348
Byproducts	$0 per lb of Niacinamide		$0
Utilities	$0.17 per lb of Niacinamide		$4,590,451
Total Variable Costs		**$**	**100,812,627**

Fixed Costs

Fixed costs include those incurred by the process but are not based on the amount of product produced from the plant. These include salaries and benefits, overhead operation costs, insurance, taxing, and maintenance cost for the equipment and the plant itself. Table H3 below outlines the total fixed costs of the project.

Table I3. Summary of Fixed Cost

Fixed Cost Summary			
Operations			
	Direct Wages and Benefits	$	364,000
	Direct Salaries and Benefits	$	54,600
	Operating Supplies and Services	$	21,840
	Technical Assistance to Manufacturing	$	-
	Control Laboratory	$	-
	Total Operations	**$**	**440,440**
Maintenance			
	Wages and Benefits	$	1,998,999
	Salaries and Benefits	$	499,750
	Materials and Services	$	1,998,999
	Maintenance Overhead	$	99,950
	Total Maintenance	**$**	**4,597,698**
Operating Overhead			
	General Plant Overhead:	$	207,132
	Mechanical Department Services:	$	70,016
	Employee Relations Department:	$	172,124
	Business Services:	$	215,884
	Total Operating Overhead	**$**	**665,156**
Property Taxes and Insurance			
	Property Taxes and Insurance:	$	888,444
Other Annual Expenses			
	Rental Fees (Office and Laboratory Space):	$	-
	Licensing Fees:	$	-
	Miscellaneous:	$	-
	Total Other Annual Expenses	**$**	**-**
Total Fixed Costs		**$**	**6,591,738**

Working Capital

Working capital is the sum of cash reserves, inventory, and accounts receivable minus accounts payable. Accounts payable, accounts receivable, and cash reserves are all assumed to be 30 days' worth. Seven days of MPDA, the raw material, is stored on site while two days' worth of the product, niacinamide, is stored at the plant site as well. A summary of the working capital for the first three years of actual plant operation is given below. The total capital investment, based on previous assumptions and calculations, is around $54,105,000.

Table I4. Summary of Working Capital

Working Capital							
			2014		2015		2016
	Accounts Receivable	$	4,540,774	$	2,270,387	$	2,270,387
	Cash Reserves	$	413,588	$	206,794	$	206,794
	Accounts Payable	$	(3,204,227)	$	(1,602,113)	$	(1,602,113)
	Niacinamide Inventory	$	302,718	$	151,359	$	151,359
	Raw Materials	$	708,037	$	354,018	$	354,018
	Total	**$**	**2,760,890**	**$**	**1,380,445**	**$**	**1,380,445**
	Present Value at 15%	*$*	*2,400,774*	*$*	*1,043,815*	*$*	*907,665*
Total Capital Investment				**$**	**54,105,125**		

Cash Flow and Profitability Analysis

Profitability and feasibility of the project are based on several measures, including return on investment (ROI), investor's return on investment (IRR), net present value (NPV), and the depreciation of the plant over the 20 year lifetime. As a base case, the plant has allocated 1 year for design, 1 year for construction, and 18 years of operating the plant. Based on this operation schedule, after the third production year, the ROI is 11.09% whereas the IRR is 16.82%, and the NPV, assuming 15% discount rate, is $4,932,800 at the end of the 20 year period. The table below summarized the cash flow sheet for the 20 year lifetime of the plant.

Table I6. Summary of Cash Flow

	Cash Flow Summary														
Year	Percentage of Design Capacity	Product Unit Price	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs	Total Costs	Depreciation	Depletion Allowance	Taxible Income	Taxes	Net Earnings	Cash Flow	Cumulative Net Present Value at 15%
2013	0%		-	-	-	-	-	-	-	-	-	-	-	-	-
2014	0%		-	(49,752,900)	(2,760,900)	-	-	-	-	-	-	-	-	(52,513,761)	(45,664,100)
2015	45%	$4.43	55,246,082	-	(1,380,400)	(45,365,700)	(6,591,738)	(51,957,420)	(8,884,400)	-	(5,595,780)	2,070,400	(3,525,341)	3,978,655	(42,655,700)
2016	68%	$4.52	84,526,505	-	(1,380,400)	(69,409,500)	(6,723,573)	(76,133,067)	(14,215,100)	-	(5,821,668)	2,154,000	(3,667,651)	9,167,010	(36,628,200)
2017	90%	$4.61	114,956,047	-	-	(94,396,900)	(6,858,044)	(101,254,956)	(8,529,100)	-	5,172,027	(1,913,700)	3,258,377	11,787,441	(29,888,700)
2018	90%	$4.70	117,255,168	-	-	(96,284,800)	(6,995,205)	(103,280,055)	(5,117,400)	-	8,857,674	(3,277,300)	5,580,335	10,697,773	(24,570,100)
2019	90%	$4.80	119,600,271	-	-	(98,210,500)	(7,135,109)	(105,345,656)	(5,117,400)	-	9,137,177	(3,380,800)	5,756,421	10,873,860	(19,869,000)
2020	90%	$4.89	121,992,277	-	-	(100,174,800)	(7,277,812)	(107,452,569)	(2,558,700)	-	11,980,988	(4,433,000)	7,548,022	10,106,742	(16,069,500)
2021	90%	$4.99	124,432,122	-	-	(102,178,300)	(7,423,368)	(109,601,621)	-	-	14,830,501	(5,487,300)	9,343,216	9,343,216	(13,015,200)
2022	90%	$5.09	126,920,765	-	-	(104,221,800)	(7,571,835)	(111,793,653)	-	-	15,127,111	(5,597,000)	9,530,080	9,530,080	(10,306,100)
2023	90%	$5.19	129,459,180	-	-	(106,306,300)	(7,723,272)	(114,029,526)	-	-	15,429,654	(5,709,000)	9,720,682	9,720,682	(7,903,300)
2024	90%	$5.30	132,048,364	-	-	(108,432,400)	(7,877,737)	(116,310,117)	-	-	15,738,247	(5,823,200)	9,915,095	9,915,095	(5,772,100)
2025	90%	$5.40	134,689,331	-	-	(110,601,000)	(8,035,292)	(118,636,319)	-	-	16,053,012	(5,939,600)	10,113,397	10,113,397	(3,881,900)
2026	90%	$5.51	137,383,117	-	-	(112,813,000)	(8,195,998)	(121,009,046)	-	-	16,374,072	(6,058,400)	10,315,665	10,315,665	(2,205,300)
2027	90%	$5.62	140,130,780	-	-	(115,069,300)	(8,359,918)	(123,429,227)	-	-	16,701,553	(6,179,600)	10,521,979	10,521,979	(718,200)
2028	90%	$5.73	142,933,395	-	-	(117,370,700)	(8,527,116)	(125,897,811)	-	-	17,035,584	(6,303,200)	10,732,418	10,732,418	600,700
2029	90%	$5.85	145,792,063	-	-	(119,718,100)	(8,697,658)	(128,415,767)	-	-	17,376,296	(6,429,200)	10,947,066	10,947,066	1,770,600
2030	90%	$5.96	148,707,905	-	-	(122,112,500)	(8,871,612)	(130,984,083)	-	-	17,723,822	(6,557,800)	11,166,008	11,166,008	2,808,200
2031	90%	$6.08	151,682,063	-	-	(124,554,700)	(9,049,044)	(133,603,764)	-	-	18,078,298	(6,689,000)	11,389,328	11,389,328	3,728,500
2032	90%	$6.21	154,715,704	-	5,521,800	(127,045,800)	(9,230,025)	(136,275,840)	-	-	18,439,864	(6,822,700)	11,617,115	17,138,894	4,932,800

J. SENSITIVITY ANALYSES

After the base case for the process was determined, detailed analysis into the profitability of the plant as dependent on variables estimated in the overall NPV of the plant was completed. Many sensitivity analyses were performed to accurately predict how the plant's value and capacity may change as a function of pricing.

Product Price and Variable Costs

The most important sensitivity analysis looks at the effect of varying the annual variable cost and the product price. The cost of niacinamide may vary slightly since the feedstock to this process is a byproduct of another manufacturing process: the production of nylon-6,6; therefore, a sensitivity analysis is conducted to determine how the results would change with price fluctuations of niacinamide. The cost of this feedstock was varied from $2.22 to $6.65 per pound, which is ± 50% of the input value for the estimated cost of bulk niacinamide. To account for variations in the total operating and variable costs associated with the plant, the variable cost is assumed to also be ± 50% of the input value. These prices both increase by 2% with inflation and the analysis is done for the first year of production only. The table following illustrates the IRR for these variable costs.

Table J.1. Sensitivity Analysis of IRR towards niacinamide Price and Variable Cost

Product Price	Variable Costs: $50,406,314	$60,487,576	$70,568,839	$80,650,102	$90,731,365	$100,812,627	$110,893,890	$120,975,153	$131,056,416	$141,137,678	$151,218,941
$2.22	1.38%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$2.66	19.39%	5.82%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.10	31.05%	21.42%	9.23%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.55	40.94%	32.56%	23.31%	12.08%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$3.99	49.90%	42.19%	34.01%	25.08%	14.57%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$4.43	58.24%	50.96%	43.39%	35.40%	26.75%	16.82%	2.98%	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$4.88	66.10%	59.15%	51.99%	44.56%	36.74%	28.34%	18.87%	6.60%	Negative IRR	Negative IRR	Negative IRR
$5.32	73.58%	66.89%	60.04%	52.99%	45.68%	38.03%	29.86%	20.78%	9.56%	Negative IRR	Negative IRR
$5.76	80.75%	74.27%	67.66%	60.90%	53.96%	46.78%	39.28%	31.31%	22.56%	12.13%	Negative IRR
$6.20	87.65%	81.35%	74.94%	68.42%	61.75%	54.91%	47.84%	40.48%	32.70%	24.24%	14.42%
$6.65	94.32%	88.17%	81.93%	75.60%	69.15%	62.57%	55.83%	48.88%	41.65%	34.04%	25.84%

As seen in the table, the current price of niacinamide can produce a positive IRR. However, as the cost of the variable costs increase, the IRR decreases with respect to a constant product price. Additionally as the cost of the product decreases, IRR becomes negative relatively quickly, assuming the variable cost calculated previously. This trends as expected for general chemical engineering process plants.

Feedstock Price

Feedstock prices for MPDA are based on the scaling of chemicals from specialty suppliers. Assuming that the cost is about 10 times less expensive than small quantities, the cost is $6.80 per pound of MPDA. However, due to fluctuations in the production of nylon-6,6 (where MPDA is a byproduct) the price of MPDA may change dependent on the current nylon-6,6 production market. To account for these changes, the price of MPDA was varied ±10% of the current projected cost. Outlined in the table below are the findings.

Table J2. Summary of ROI and IRR for MPDA Price Changes

MPDA Price ($/lb)	**2.03**	**2.25**	**2.50**	**2.78**	**3.09**	**3.40**	**3.74**	**4.11**	**4.53**	**4.98**
IRR	40.97%	36.47%	31.20%	24.86%	**16.82%**	6.31%	Negative	Negative	Negative	Negative
ROI	40.04%	34.04%	27.29%	19.68%	**11.09%**	2.36%	-7.42%	-18.40%	-30.74%	-44.65%

As evident by the deviation from the projected price of MPDA chart, if the cost of MPDA increases by more than 20% the current cost, this process will have a negative return on the investment, making it an undesirable process to invest in. However, if the cost of MPDA decreases, the return on investment increases by almost ten percent as the cost of the feedstock decreases by ten percent. Close to the "breaking even" point for this process is a fifteen percent increase from the current calculated price for MPDA. Here, the cost IRR and ROI are very close to 0% for both.

Based on this analysis, this project is highly sensitive to the feedstock prices for MPDA , due in part because MPDA is generally the most expensive and the only large-scale feedstock needed for the process to producing niacinamide.

Inflation Rate

The inflation rate used for the previous base case calculations was determined using predictions for the next few years. Since this project continues for 20 years, though, the inflation rate may change year to year. If this changes, the overall IRR, ROI, and NPV will change accordingly due to the increase in the cost of the plant and the feedstock. Yet at the same time the selling price of the product will also increase. Below is a table that summarizes the overall IRR, ROI, and NPV that occurs when the inflation rate of the total system changes.

Table J3. Summary of ROI, IRR, and NPV for Inflation Rate Changes

Inflation Rate (%)	**0**	**1**	**2**	**3**	**4**	**5**	**6**
IRR	15.04%	15.93%	**16.82%**	17.71%	18.61%	19.52%	20.42%
ROI	10.49%	10.79%	**11.09%**	11.40%	11.71%	12.03%	12.34%
NPV	$ 92,600	$ 2,413,200	**$4,932,800**	$ 7,671,200	$ 10,650,500	$ 13,895,000	$ 17,431,600

Currently, the inflation rate was selected to be 2%. When the inflation rate decreases, however, the overall NPV and rate of returns decrease. When the inflation rate is increased, the net present value and rate of return on the investment increases. This trend appears because the value of the equipment purchased increases as the years progress; therefore, over a longer period of time, the net present value of the process would be greater with a greater inflation rate due to the net worth of the equipment present in the process. The return of investment changes by 0.3% when the inflation rate changes by a percent in either direction. Although the ROI doesn’t change significantly between the inflation rates, the NPV does change drastically, increasing as the inflation rate increases. With this, it is evident that the ROI, IRR, and NPV of the process is significantly dependent on the inflation rate of the entire system.

MPDA to Niacinamide Ratio

Currently, the percent conversion the authors have used are very ideal estimates. In this case, the yield per pound of MPDA will change with a decrease in the conversion of each reaction vessel. To account for this, a sensitivity analysis of the pound MPDA versus pound niacinamide was analyzed. The table below illustrates the drastic effects that MPDA has on the overall IRR, ROI, and NPV of the process.

Table J4. Summary of lb MPDA vs. lb Niacinamide

lb MPDA/lb Niacinamide	**0.958**	**1.054**	**1.159**	**1.275**
IRR	**16.82%**	6.31%	Negative IRR	Negative IRR
ROI	**11.09%**	2.36%	-7.42%	-18.40%
NPV	**$ 4,932,800**	$ (19,717,000)	$ (46,831,800)	$ (76,658,100)

Based on these calculations, the amount of MPDA per pound of niacinamide greatly influences the ROI, IRR, and NPV. If the process as a whole is decreased just 10%, the NPV becomes negative after 20 years rather than a positive as seen with the current calculations. Therefore the calculations made previously in the process, wherein the reactors had very large conversion rates, would significantly affect the IRR, ROI, and NPV of the entire process if conversions of these magnitude could not be reached.

VI. CONCLUSIONS AND RECOMMENDATIONS

Overall, the base-case design for the production of niacinamide from MPDA, a byproduct of nylon-6,6 manufacturing, was designed, analyzed, and priced under a variety of economic considerations. The entire system provides a green process to producing niacinamide in relatively high purity, around 97.7%. After analyzing the base-case design and economic analysis of this process, it has been found that this venture will be profitable within 14 years, with an ROI of 11.09% and an IRR of 16.82% after the third year. The NPV after 20 years is $4,932,800. Since the NPV is positive when taken to have a 20 year lifetime, it may be a profitable investment if investors do not require an immediate return on the investment. However, since there are more pieces of equipment and research to be done to provide niacinamide that is of competitive purity, it may be unwise to continue investing time and money to pursue this process, unless the capital investment available is relatively large.

If the process were to be built upon and improved, the return on investment may outweigh the cost of the initial investment. With an increased purity, and therefore an increased selling price for niacinamide, the process would yield a better return on the initial investment earlier in the project lifetime. Also due to the increases in federal regulations over the past few years, it is difficult to predict what future regulations may entail. Regulations for water and air quality will increase, leading to issues surrounding the possible leakage of harsh, carcinogenic chemicals produced as intermediates in previous pathways to niacinamide production. In this case an increase in regulations would benefit this process, favoring it over the conventional production process. Since the process requires very little toxic intermediates and relatively simple exhaust gas and waste water clean-up, federal regulations would make other less environmentally friendly processes more costly because of increased costs in cleaning streams.

The significant obstacle to commercialization of this process is the large capital investment. In reference to the Lonza process, this company is able to afford this new technology because they have already captured a market for niacinamide, being the world's leading producer of niacin. In addition, around 2005 the relationship between this company and China was relatively good. They seized the opportunity to create a process that would use government incentives and regulations to benefit the overall process design and cost. However, if no infrastructure has been developed beforehand, this project would be an extremely risky investment venture.

Without the variable costs and large degree of necessary heat integration, the process may have been most cost effective. If the process was able to use less equipment and utilities, the overall cost of the process may yield better returns on investment since the general idea not only decreases the amount of CO and CO_2 emitted to the atmosphere, but it also eliminates harmful chemicals that are considered carcinogens. To increase the yield and purity of this product, more distillation columns, extraction units, and separation processes must be implemented. After the 14 years it takes to gain a return on the investment, the technology available for the production of niacinamide will also have changed drastically. This makes analyzing the profitability and lifetime of the plant difficult.

This process is not recommended for continued design research. In 1999, Lonza ventured to set up its first niacinamide production plant in China because the North American and European markets for nicotinates were "saturated" (Tremblay, 1999). At that time the Southeast Asian market was expected to grow 8 to 10% annually (Tremblay, 1999). However, in the past ten years, a great number of production plants, especially in India, have emerged, utilizing a different green process to niacin production. This would further saturate the market making it more difficult to design a process where the technology may already be outdated. As seen in Table J4, the relatively low return on investment, the potentially large fluctuations in the cost of MPDA and subsequent decrease in return, and the impedingly large amount of capital are all unfavorable to a new company. The technology used in this process may already be surpassed by another technology not yet commercially available, especially due to the biocatalyst present in the system. In conclusion, it has been determined that this process is better than the classical method of niacin production using permanganate, chromic acid, and other metal oxides. However, it is not recommended to use this process for a company that does not already have a portion of the niacin market.

VII. Acknowledgments

The authors would like to thank Mr. Leonard Fabiano, for his help with the Dowtherm system and his knowledge of industrial experience. He should also be thanked for taking the time out of his busy schedule to meet with the authors to discuss issues pertaining to the project.

The authors would also like to thank Dr. Sean Holleran for bringing his experience in chemical engineering principles and advice to structuring and formatting the design. We also wish to thank Dr. Holleran for his constant efforts to keep the group on track towards completion of the project.

In addition, the numerous consultants that helped through the entire project should also be recognized. The authors wish to thank Mr. Adam Brostow from Air Products, Mr. David Kolesar from Dow Chemical, Mr. John Wismer from Arkema, and Mr. Richard Bockrath for providing additional consulting information when needed. Finally the authors would also like to thank Dr. Daeyeon Lee for his help in understanding the separation processes associated with the process design at the beginning of the project.

VIII. REFERENCES

(FEEDAP), EFSA Panel on Additives and Products or Substances used in Animal Feed. (2012). Scientific Opinion on the safety and efficacy of niacin (nicotinic acid and nicotinamide) as a feed additive for all animal species based on a dossier submitted by Lonza Benelux BV. *EFSA Journal 2012, 10*(7), 19. doi: doi:10.2903/j.efsa.2012.2788

Abe, T., Itou, K., Sasaki, K., Watanabe, S., Asano, T., Abe, G., & Ito, K. WO200153253-A; WO200153253-A1; JP2001270857-A; EP1167345-A1; CN1319585-A; KR2001102572-A; US2003104586-A1; TW553922-A; CN1194961-C; KR482686-B; EP1167345-B1; DE60133691-E; DE60133691-T2; US7700330-B2; JP4959059-B2.

Abuschinow, M., Hussain, D., & Wu, K. (2009). *Hydrogenation of Maleic Acid to Tetrahydrofuran.* B.S.E. Chemical Biomolecular Engineering Senior Design Report, University of Pennsylvania. Retrieved from http://repository.upenn.edu/cbe_sdr/1/

Acros Organics. (2011, May 9). *3-Cyanopyridine* [Material Safety Data Sheet]. Retrieved from http://www.acros.com/Ecommerce/msds.aspx?PrdNr=11086&Country=NULL&Language=EN

Alternative Fuels Data Center, U.S. Department of Energy. (March 29, 2013). Renewable Natural Gas (Biogas). Retrieved from http://www.afdc.energy.gov/fuels/emerging_biogas.html

Andersen, T. M. (Accessed March 27, 2012). CIP Cycle Development: Manual to Automated Cleaning, McFlusion Inc. Retrieved from http://www.morkusa.com/images/CIP_Cycle_Development_INTERPHEX_060120.pdf

Askari, Aboalfaz, Karimi, Hajir, Rahimi, M. Reza, & Ghanbari, Mehdi. (2012). Simulation and Modeling of Catalytic Reforming Process. *Petroleum & Coal, 54*(1), 76-84.

B, S. Kumar A and B. V. Babu. (2008). Process Intensification of Nicotinic Acid Production via Enzymatic Conversion using Reactive Extraction. *Chemical and Biochemical Engineering Quarterly*.

Bartholomew, Calvin H., & Farrauto, Robert J. (2005). Hydrogen Production and Synthesis Gas Reactions *Fundamentals of Industrial Catalytic Processes* (pp. 339-486): John Wiley & Sons, Inc.

Beschke, H., Friedrich, H., & Heilos, J. JP93000096-B2; EP59414-B1; EP59414-A2; EP59414-A; DE3107755-A; JP57156038-A; CA1164437-A; US4447612-A; EP59414-B; DE3267083-G; SU1189327-A; JP93000096-B.

BioSNG. (2007, June 4, 2007) Retrieved March 25, 2013, from http://www.biosng.com/

Bondareva, V. M., Ovchinnikova, E. V., & Andrushkevich, T. V. (2008). Kinetics of β-picoline oxidation to nicotinic acid over vanadia-titania catalyst. 3. The oxidation of nicotinic acid. *Reaction Kinetics and Catalysis Letters, 94*(2), 327-335. doi: 10.1007/s11144-008-5356-9

Cantarella, L., Gallifuoco, A., Malandra, A., Martínková, L., Spera, A., & Cantarella, M. (2011). High-yield continuous production of nicotinic acid via nitrile hydratase–amidase cascade reactions using cascade CSMRs. *Enzyme and Microbial Technology, 48*(4–5), 345-350. doi: http://dx.doi.org/10.1016/j.enzmictec.2010.12.010

Cantarella, M., Cantarella, L., Gallifuoco, A., Spera, A., & Martínkovà, L. (2012). Nicotinic acid bio-production by Microbacterium imperiale CBS 489-74: Effect of 3-cyanopyridine and temperature on amidase activity. *Process Biochemistry, 47*(7), 1192-1196. doi: http://dx.doi.org/10.1016/j.procbio.2012.03.010

Carlson, L. A. (2005). Nicotinic acid: the broad-spectrum lipid drug. A 50th anniversary review. *Journal of Internal Medicine, 258*(2), 94-114. doi: 10.1111/j.1365-2796.2005.01528.x

Chesalov, Yu A., Ovchinnikova, E. V., Chernobay, G. B., Popova, G. Ya, & Andrushkevich, T. V. (2010). Mechanism of the oxygen involvement in nicotinic acid formation under β-picoline oxidation on V-Ti-O catalyst. *Catalysis Today, 157*(1–4), 39-43. doi: http://dx.doi.org/10.1016/j.cattod.2010.01.065

Chuck, R. J., Zacher, U., Roderick, J. C., Chaque, R. J., & Cahel, U. EP919548-A; EP919548-A1; CZ9803816-A3; SK9801581-A3; NO9805489-A; JP11217373-A; CA2253615-A1; CN1222511-A; US6077957-A; KR99045503-A; HU9802719-A1; NO311887-B1; US6376677-B1; TW495503-A; MX9809833-A1; IL127201-A; EP919548-B1; DE59811380-G; ES2221110-T3; SK284427-B6; MX230893-B; CZ296894-B6; CZ296940-B6; HU225089-B1; CN1272321-C; SK285375-B6; CN1900062-A; KR611542-B1; HU226169-B1; CA2253615-C; MX251718-B; CN100478332-C; IN187776-B; JP4586214-B2.

Chuck, Roderick. (2005). Technology development in nicotinate production. *Applied Catalysis A: General, 280*(1), 75-82. doi: http://dx.doi.org/10.1016/j.apcata.2004.08.029

Chuck, Roderick. (2009). Green Sustainable Chemistry in the Production of Nicotinates *Sustainable Industrial Chemistry* (pp. 541-550): Wiley-VCH Verlag GmbH & Co. KGaA.

DiCosimo, Robert. (2006). Nitrilases and Nitrile Hydratases *Biocatalysis in the Pharmaceutical and Biotechnology Industries*: CRC Press.

Dieudonné, Batsy, Charles, Solvason, Norm, Sammons, Virginie, Chambost, David, II, Mario, Eden, . . . Paul, Stuart. (2012). Product Portfolio Selection and Process Design for the Forest Biorefinery *Integrated Biorefineries* (pp. 3-36): CRC Press.

Doble, Mukesh. (2006). Avoid the pitfalls of bioprocess development. *Chemical Engineering Progress, 102,* 34 - 41.

DuPont. (2011, November 1). *DOWTHERM A* [Material Safety Data Sheet]. Retrieved from http://msdssearch.dow.com/PublishedLiteratureDOWCOM/dh_08a5/0901b803808a5b98.pdf?filepath=heattrans/pdfs/noreg/176-01463.pdf&fromPage=GetDoc

DuPont. (1997, March). *DOWTHERM A Heat Transfer Fluid* [Product Technical Data]. Retrieved from http://msdssearch.dow.com/PublishedLiteratureDOWCOM/dh_0030/0901b803800303cd.pdf?filepath=/heattrans/pdfs/noreg/176-01337.pdf&fromPage=GetDoc

DuPont. (2011, September 12). SUVA® 134a refrigerant [Material Safety Data Sheet]. Retrieved from http://msds.dupont.com/msds/pdfs/EN/PEN_09004a358054797d.pdf

Elshout, Ray. (2010). Hydrogen Production by Steam Reforming. *Chemical Engineering, May 2010*, 34-38.

EPA Emergency Management (2004). Appendix F: Supplemental Risk Management Program Guidance for Wastewater Treatment Plants. General Risk Management Program Guidance, EPA.

Feedinfo News Services (July 16, 2012). Interview: Vitamin B3 - Jubilant Well-Positioned to Cater for Global Demand. Retrieved from http://www.feedinfo.com/console/PageViewer.aspx?page=3098557

Fermeglia M., Longo, G., and Letitia, T (2007). A Hierarchical approach for the estimation of environmental impact of a chemical process: from molecular modeling to process simulation. *European Symposium on Computer Aided Process Engineering,* 5. Retrieved from http://institute.unido.org/documents/M8_LearningResources/ICS/24.%20A%20Hierarchical%20Approach%20for%20the%20Estimation%20of%20Environmental%20Impact%20of%20a%20Chemical%20Process-%20from%20Molecular%20Modeling%20to%20Process%20Simulation.pdf

Gangadharan, P., Zanwar, A., Zheng, K., Gossage, H. (April 20120). Sustainability assessment of polygeneration processes based on syngas derived from coal and natural gas, *Computers & Chemical Engineering, 39,* (105-117). doi: http://dx.doi.org/10.1016/j.compchemeng.2011.10.006

Gay, M., Pope, B., & Wharton, J. (2011). *Propylene from Biomass.* B.S.E. Chemical Biomolecular Engineering Senior Design Report, University of Pennsylvania. Retrieved from http://repository.upenn.edu/cbe_sdr/23/

Ghisalba, Oreste, Meyer, Hans-Peter, Wohlgemuth, Roland, & Flickinger, Michael C. (2009). Industrial Biotransformation *Encyclopedia of Industrial Biotechnology: Bioprocess, Bioseparation, and Cell Technology* (pp. 1-34): John Wiley & Sons, Inc.

Gonçalves, Elsa M., & Minas da Piedade, Manuel E. (2012). Solubility of nicotinic acid in water, ethanol, acetone, diethyl ether, acetonitrile, and dimethyl sulfoxide. *The Journal of Chemical Thermodynamics, 47*(0), 362-371. doi: http://dx.doi.org/10.1016/j.jct.2011.11.023

Heveling, J., Armbruster, E., Siegrist, W., & Slegrist, W. WO9422824-A; EP691955-A; WO9422824-A1; AU9465376-A; ZA9402303-A; TW239129-A; FI9504660-A; NO9503896-A; BR9405915-A; CH686135-A5; EP691955-A1; SK9501226-A3; CZ9502542-A3; JP8510447-W; EP691955-B1; AU678232-B; DE59402925-G; HU72028-T; ES2104377-T3; US5714610-A; NO303937-B1; IL109173-A; RU2127726-C1; HU217780-B; MX192306-B; CZ287321-B6; SK281702-B6; KR276748-B; RO117914-B1; CA2159586-C; FI112473-B1; JP3520519-B2; RO121267-B1.

Huang, J.-C., & Shang, C. (2006). Air Stripping. In L. Wang, Y.-T. Hung & N. Shammas (Eds.), *Advanced Physicochemical Treatment Processes* (Vol. 4, pp. 47-79): Humana Press.

Invista. (2012, March 15). *DYTEK® 2-Methylpentamethylenediamine (MPMD) (DYTEK® A amine)* [Technical Data Sheet]. Retrieved from http://www.dytek.invista.com/documents/tds/DYTEK%C2%AE%20A%20Amine%20Technical%20Data%20Sheet.pdf

Invista. (2012). Global Locations. Retrieved from http://www.invista.com/en/inside-invista/locations.html.

Iranshahi, Davood, Bahmanpour, Ali Mohammad, Pourazadi, Ehsan, & Rahimpour, Mohammad Reza. (2010). Mathematical modeling of a multi-stage naphtha reforming process using novel thermally coupled recuperative reactors to enhance aromatic production. *International Journal of Hydrogen Energy, 35*(20), 10984-10993. doi: http://dx.doi.org/10.1016/j.ijhydene.2010.07.077

Ishige, Takeru, Honda, Kohsuke, & Shimizu, Sakayu. (2005). Whole organism biocatalysis. *Current Opinion in Chemical Biology, 9*(2), 174-180. doi: http://dx.doi.org/10.1016/j.cbpa.2005.02.001

Jess, A., & Kern, C. (2009). Modeling of Multi-Tubular Reactors for Fischer-Tropsch Synthesis. *Chemical Engineering & Technology, 32*(8), 1164-1175. doi: 10.1002/ceat.200900131

Joseph, Abhinav, Bernardes, Carlos E. S., & Minas da Piedade, Manuel E. (2012). Heat capacity and thermodynamics of solid and liquid pyridine-3-carboxylic acid (nicotinic acid) over the temperature range 296 K to 531 K. *The Journal of Chemical Thermodynamics, 55*(0), 23-28. doi: http://dx.doi.org/10.1016/j.jct.2012.06.010

Lantec Products Inc. (2004). Ammonia Removal - Water Purification in Packed Bed Air Stripper. *Case Study*. Retrieved from http://www.lantecp.com/casestudy/cs49.pdf

Lonza Engineering, Ltd. (2012). Lonza Engineering. In L. E. Ltd (Ed.). http://www.lonza.com: Lonza.

Lonza Group, Ltd. (2011). Lonza Activities 2010. Basel, Switzerland. Retrieved from http://www.lonza.com/about-lonza/media-center/news/2011/lonza-celebrates-40-years-as-leading-producer-of-vitamin-b3.aspx

Lonza Group, Ltd. (2012). Lonza Annual Report 2011. Retrieved from http://ir2.flife.de/data/lonza1/igb_html/index.php?bericht_id=1000003&lang=ENG

Lonza Group, Ltd. (2012). Plant Safety, Explanation of Customer Needs Clusters, Niacin and Niacinamide Differentiation. Retrieved from http://www.lonza.com/products-services/nutrition/animal-nutrition/niacin-niacinamide-differentiation.aspx

Ludwig. P.E, Ernest E. (2001). Chapter 11 Refrigeration systems. In E. E. Ludwig. P.E (Ed.), *Applied Process Design for Chemical & Petrochemical Plants* (Vol. Volume 3, pp. 289-367): Gulf Professional Publishing.

Martin, A., Janke, C., & Kalevaru, V. N. (2010). Ammoxidation of 3-picoline to nicotinonitrile over VPO catalysts. *Applied Catalysis A: General, 376*(1–2), 13-18. doi: http://dx.doi.org/10.1016/j.apcata.2009.09.043

Mathew, C. D., Nagasawa, T., Kobayashi, M., & Yamada, H. (1988). Nitrilase-Catalyzed Production of Nicotinic Acid from 3-Cyanopyridine in Rhodococcus rhodochrous J1. *Appl Environ Microbiol, 54*(4), 1030-1032.

Meyer, H. P. & Ruesing, M. (2008, April). *Examples of bioprocesses for the production of nutraceuticals* [PowerPoint slides]. Retrieved from Lonza Ltd, Visp and Basel, Switzerland website: http://bio.lonza.com/uploads/tx_mwaxmarketingmaterial/Lonza_PowerpointSlidesCollections_HPM_MR_2008_Chicago_Neutraceuticals.pdf

Murphy, Annabel C. (2011). Metabolic engineering is key to a sustainable chemical industry. *Natural Product Reports, 28*(8), 1406-1425.

Perry, R. & Green, D. (2008). *Perry's Chemical Engineers' Handbook*. New York: McGraw-Hill.

Pharmaceutical-technology.com. (2011). Lonza Niacinamide Production Facility, China. Retrieved from http://www.pharmaceutical-technology.com/projects/lonza-niacinamide-production-guangzhou/

Phillips, J. (1995). *Control and pollution prevention options for ammonia emissions.* Research Triangle Park, NC: Control Technology Center, U.S. Environmental Protection Agency.

Nagasawa, T., & Yamada, H. EP307926-B; EP307926-A2; DD274631-B; JP94055148-B; EP307926-A; NO8804114-A; BR8804804-A; DK8805166-A; FI8804279-A; PT88540-A; HU50215-T; JP2000470-A; CN1032436-A; DD274631-A; CA1298222-C; RO101578-A; EP307926-B1; DE3877869-G; ES2043752-T3; JP94055148-B2; NO175489-B; US5334519-A; FI93858-B; SU1838416-A3; KR134094-B1; DK174516-B.

Ohio EPA. (1993) "Wet Scrubbers". *Ohio EPA's Operation and Maintenance Guidelines for Air Pollution Control Equipment*. Retrieved from http://www.epa.state.oh.us/portals/27/engineer/eguides/scrubbers.pdf

Ovchinnikova, E. V., Chumachenko, V. A., Vernikovskaya, N. V., Kashkin, V. N., & Andrushkevich, T. V. (2010). A study of nicotinic acid synthesis on a pilot installation and its simulation. *Russian Journal of Applied Chemistry, 83*(5), 846-853. doi: 10.1134/s1070427210050162

Ovchinnikova, E. V., Vernikovskaya, N. V., Andrushkevich, T. V., & Chumachenko, V. A. (2011). Mathematical modeling of β-picoline oxidation to nicotinic acid in multitubular reactor: Effect of the gas recycle. *Chemical Engineering Journal, 176–177*(0), 114-123. doi: http://dx.doi.org/10.1016/j.cej.2011.06.047

Ovchinnikova, ElenaV, Popova, GalinaYa, & Andrushkevich, TamaraV. (2009). Kinetics of oxidation of β-picoline to nicotinic acid over vanadia-titania catalyst. 4. Kinetic model. *Reaction Kinetics and Catalysis Letters, 96*(1), 91-100. doi: 10.1007/s11144-009-5461-4

Powell, K. A., Ramer, S. W., Del Cardayre, S. B., Stemmer, W. P., Tobin, M. B., Longchamp, P. F., & Huisman, G. W. (2001). Directed Evolution and Biocatalysis. *Angew Chem Int Ed Engl, 40*(21), 3948-3959.

Raja, Robert, Adams, Richard D., Blom, Douglas A., Pearl, William C., Gianotti, Enrica, & Thomas, John Meurig. (2009). New Catalytic Liquid-Phase Ammoxidation Approach to the Preparation of Niacin (Vitamin B3). *Langmuir, 25*(13), 7200-7204. doi: 10.1021/la900803a

Rutledge, B. (April 2005). California Biogas Industry Assessment White Paper, *WetStart-CALSTART*, 3-27. Retrieved from http://www.calstart.org/Libraries/Publications/California_Biogas_Industry_Assessment_White_Paper.sflb.ashx

Schmid, A., Dordick, J. S., Hauer, B., Kiener, A., Wubbolts, M., & Witholt, B. (2001). Industrial biocatalysis today and tomorrow. *Nature, 409*(6817), 258-268.

Seay, J. and Gish, J. (2010) Educational Module: A Sustainable Design Project for the Process Separations Class, *University of Kentucky*. Retrived from http://lcs.syr.edu/centers/SustainableEngineering/modules/10-21_Seay.pdf

Seider, W. D., Seader, J. D., Lewin, D. R., Widagdo, S. (2009) Product and Process Design Principles: Synthesis, Analysis and Design, 3rd Edition, John Wiley & Sons, Inc., Hoboken, NJ, USA.

Sembaev, D. C., Ivanovskaya, F. A., Guseinov, E. M., Chuck, R. J., Sembaev, D., Ivanovskaya, F., . . . Chuck, J. R. WO9532055-A; WO9532055-A1; AU9527356-A; NO9604989-A; EP760709-A1; FI9604650-A; SK9601497-A3; CZ9603384-A3; BR9507744-A; US5698701-A; HU76438-T; AU688059-B; JP10504489-W; KR97703199-A; EP760709-B1; DE69509519-E; ES2130621-T3; MX9605500-A1; RU2123880-C1; MX190865-B; CN1150393-A; CZ288617-B6; SK282311-B6; NO313272-B1; RO118052-B1; KR361060-B; HU222377-B1; CN1087190-C; CA2188797-C; JP3941121-B2; FI120292-B1.

Sharma, Nitya Nand, Sharma, Monica, Kumar, Harish, & Bhalla, Tek Chand. (2006). Nocardia globerula NHB-2: Bench scale production of nicotinic acid. *Process Biochemistry, 41*(9), 2078-2081. doi: http://dx.doi.org/10.1016/j.procbio.2006.04.007

Sie, S.T. (April 30, 2001). Consequences of catalysts deactivation for process design and operation. *Applied Catalysis A: General*, *212*, p.129-151. http://dx.doi.org/10.1016/S0926-860X(00)00851-6

Sigma-Aldrich. (2012, December 12). *1,5-Diamino-2-methylpentane* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/329665?lang=en&region=US

Sigma-Aldrich. (2013, January 15). *3-Pyridinecarbonitrile* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/c94807?lang=en&region=US

Sigma-Aldrich. (2013, February 20). *3-Methylpiperidine* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/m73001?lang=en&region=US

Sigma-Aldrich. (2013, February 22). *3-Picoline* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/p42053?lang=en&region=US

Sigma-Aldrich. (2012, April 25). *Aluminum oxide* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/sial/11028?lang=en&region=US

Sigma-Aldrich. (2012, December 5). *Ammonia* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/294993?lang=en&region=US

Sigma-Aldrich. (2012, December 5). *Carbon Dioxide* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/295108?lang=en&region=US

Sigma-Aldrich. (2012, October 10). *Dowtherm® A* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/44570?lang=en&region=US

Sigma-Aldrich. (2012, October 29). *Ethylene* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/fluka/03484?lang=en&region=US

Sigma-Aldrich. (2012, December 5). *Hydrogen* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/295396?lang=en&region=US

Sigma-Aldrich. (2012, November 13). *Nicotinamide (Niacinamide)* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/supelco/47865u?lang=en&region=US

Sigma-Aldrich. (2012, December 5). *Nitrogen* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/295574?lang=en&region=US

Sigma-Aldrich. (2012, December 5). *Oxygen* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/295604?lang=en&region=US

Sigma-Aldrich. (2009, July 8). *ThalesNano CatCart® catalyst cartridge system, 30 mm L, 10% Pd/Al2O3* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/295604?lang=en&region=US

Sigma-Aldrich. (2012, September 9). *Vanadium(V) oxide* [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/aldrich/204854?lang=en&region=US

Sigma-Aldrich. (2012, July 3). Water [Material Safety Data Sheet]. Retrieved from http://www.sigmaaldrich.com/catalog/product/sigma/w3500?lang=en&region=US

Srinivasan, A., Chowdhury, P., & Viraraghavan, T. (2008). Air Stripping in Industrial Waste Water Treatment, in Waste Water Treatment Technologies, edited by S Vigneswaran, in Encyclopedia of Life Support Systems (EOLSS), Developed under the Auspices of the UNESCO, Eolss Publishers, Oxford ,UK, http://www.eolss.net

Sterile Processing University. (2007). Steam Sterilization. Retrieved from http://www.spdceus.com/steam_sterilization.htm

Stocking, A.J., Eylers, H.E., Wooden, M., Kavanaugh, M.C. (2000). "**Air Stripping**." *Treatment Technologies for Removal of MTBE from Drinking Water: Air Stripping, Advanced Oxidation Processes, Granular Activated Carbon, Synthetic Resin Sorbents*. Melin, Gina (Ed). MTBE Research Partnership. National Water Research Institute. Available at: http://www.nwri-usa.org/asp/BooksList.asp?id=4&main=m4&sub=s4&CtgID=12

Thomas, Stuart M., DiCosimo, Robert, & Nagarajan, Vasantha. (2002). Biocatalysis: applications and potentials for the chemical industry. *Trends in Biotechnology, 20*(6), 238-242. doi: http://dx.doi.org/10.1016/S0167-7799(02)01935-2

Tremblay, Jean-François. (1999). Lonza niacinamide plant opens in China. *Chemical & Engineering News Archive, 77*(43), 24. doi: 10.1021/cen-v077n043.p024

Trimm, D. L. (2001). The regeneration or disposal of deactivated heterogeneous catalysts. *Applied Catalysis A: General, 212*(1–2), 153-160. doi: http://dx.doi.org/10.1016/S0926-860X(00)00852-8

Tufvesson, Pär, Lima-Ramos, Joana, Nordblad, Mathias, & Woodley, John M. (2010). Guidelines and Cost Analysis for Catalyst Production in Biocatalytic Processes. *Organic Process Research & Development, 15*(1), 266-274. doi: 10.1021/op1002165

US EPA. (2001) “Air Pollution Control Technology Fact Sheet: Selective Non-Catalytic Reduction”. *Air Pollution Control Technology Handbook*. Retrieved from http://www.epa.gov/ttn/catc/dir1/fsncr.pdf

US EPA (2008). Waste Reduction Algorithm. Retrieved from http://www.epa.gov/nrmrl/std/war/sim_war.htm

Van Pelt, Sander. (2010). *The Application of Nitrile Hydratases in Organic Synthesis.* (Dissertation), Delft University of Technology. Retrieved from http://repository.tudelft.nl/view/ir/uuid:b2057153-c80d-4e32-93a4-a503389df8d9/ Institutional Repository database.

Verwijs, J.W. , Kosters, P.H.,van den Berg, H & Westerterp, K.R. (January 1995). Reactor Operating Procedures for Startup of Continuously-Operated Chemical Plants. *American Institute of Chemical Engineerings, Reactors, Kinetics and Catalysis, 41,* 148-158. Retrieved from http://doc.utwente.nl/71197/1/Verwijs95reactor.pdf

Vitamin venture sustains Asia. (1999, October 1). ICIS.com: Chemical Industry News & Chemical Market Intelligence. Retrieved from http://www.icis.com/Articles/1999/10/01/102438/vitamin-venture-sustains-asia.html

Watanabe, I., & Okumura, M. EP188316-A2; EP188316-A; JP61162193-A; FI8600058-A; CN8600062-A; SU1512488-A; JP92004873-B; US5179014-A; EP188316-B1; DE3689196-G.

Wildy, F. (2003) “Fired Heater Optimization”. AMETEK, Process Instrument, Pittsburgh, U.S.A, 1-4.

Wyssmont Turbo Dryer Advertisement - RESEARCH RESULTS. (1963). *Industrial & Engineering Chemistry, 55*(2), 83-87. doi: 10.1021/ie50638a013

Zenklusen, A., & Pianzola, D. WO2011045003-A2; US2011092710-A1; EP2319833-A1; WO2011045003-A3; CA2774888-A1; MX2012004463-A1; AU2010306132-A1; KR2012087149-A; EP2488498-A2; CN102574802-A.

IX. Appendix

A. PROBLEM STATEMENT

A Green Process to Produce Niacin
(Recommended by Leonard A. Fabiano, U. Penn)

The co-enzyme nicotinamide-adenine (NAD) and co-enzyme nicotinamide-adenine dinucleotide phosphate (NADP) are required by all living cells. They enable both the conversion of carbohydrates into energy and the metabolism of proteins and fats. Both nicotinamide and nicotinic acid (niacin) are building blocks for these co-enzymes. Niacin, the common name for a vitamin, supplements the intake of nicotinic acid in foodstuffs. Although the latter is found naturally in wheat, yeast, pork, and beef liver, synthetic niacin production has increased worldwide to significantly decrease deaths due to the vitamin deficiency disease, pellagra.

Your design team represents an engineering consulting firm that has been engaged by a potential producer of niacin. They are estimating the capital and production costs of several processes that incorporate the Lonza process to produce nicotinic acid, which involves the direct air oxidation of picoline, whose "green chemistry" is more environmentally safe for the processing plant and its surrounding area.

Reference 1 describes the methods used to produce niacin using the Lonza process. Together with the patent in reference 2, this will provide the background your team will need to begin its design. Additional information is provided in the references cited therein.

The following definition of a green process is included in [1]:

"We cannot agree that the acceptability of a process is governed solely by its cost. An economic process is not necessarily green, especially if waste treatment is ignored or neglected. An industrial process may contravene one or more green principles, and yet still make money, even if complex waste treatment adds to the costs and diminishes economic viability. But, the cost of energy today is extremely low, considering the fact that our present utilizable energy resources are limited. Thus, for a given product, the following guidelines should govern the choice of route:

Choice of feedstock (costs are relevant of course, but also total resources, energy, waste, etc., in the manufacture of the given feedstock are important factors)
Choice of reaction path (minimize energy requirements by use of selective catalysts).
Choice of catalyst (efficiency, separation from product, recycling of catalyst).
Downstream processing/unit operations (minimizing the number of stages necessary to obtain the product in the state desired by the customer).
Minimizing not only the amount of pollutants, but also the volume of waste streams (effluent off-gases and solid waste).
Recycling of auxiliary, side, and intermediate products into the process."

Your mission will include, but will not be limited to:

Determining the world market for niacin and the current production capacity worldwide.
Determining the selling price of niacin to consumers.
Based on worldwide production capacity and market consumption, deciding on the likely economic production rate. For new entries to many markets, care must be taken not to overload the markets, hurting the potential for market-share capture. A value of 5-10% increase is a typical target. Can your team determine otherwise?
Designing a facility and estimating capital and operating costs. Is there another capacity that would be more economical? Would your team propose a larger capacity to achieve these results? If so, on what basis?

Starting with a simplified process flow-sheet, are there processing improvements that you can develop? Be certain that your final process is "green" – compared to existing processes.

References

Chuck, R., "A Catalytic Green Process for the Production of Niacin" – see WDS for a copy of the unpublished paper.

Heveling et al., U. S. Patent 5,719,045, "Process for Preparing Nicotamide," Feb. 17,1998 – see WDS for a copy.

B. RELEVANT PATENTS

US005719045A

United States Patent [19]

Heveling et al.

[11] **Patent Number: 5,719,045**

[45] **Date of Patent: Feb. 17, 1998**

[54] **PROCESS FOR PREPARING NICOTINAMIDE**

[75] Inventors: **Josef Heveling**; **Erich Armbruster**, both of Naters; **Lukas Utiger**, Termen; **Markus Rohner**, Kourim; **Hans-Rudolf Dettwiler**; **Roderick J. Chuck**, both of Brig-Glis, all of Switzerland

[73] Assignee: **Lonza AG**, Gampel/Valais, Switzerland

[21] Appl. No.: **741,806**

[22] Filed: **Oct. 31, 1996**

[30] **Foreign Application Priority Data**

Nov. 1, 1995 [CH] Switzerland 3090/95

[51] **Int. Cl.**[6] **C12P 17/12**

[52] **U.S. Cl.** **435/122**; 435/129; 435/170; 435/252.1

[58] **Field of Search** 435/122, 129, 435/170, 252.1

[56] **References Cited**

U.S. PATENT DOCUMENTS

5,179,014 1/1993 Watanabe et al. 435/129
5,258,305 11/1993 Yamada et al. 435/280
5,334,519 8/1994 Yamada et al. 435/129

FOREIGN PATENT DOCUMENTS

0188316 8/1986 European Pat. Off. .
0307926 3/1989 European Pat. Off. .
WO 94/22824 10/1994 WIPO .
WO 95/32055 11/1995 WIPO .

OTHER PUBLICATIONS

Ullmann's Encyklopädie der technischen Chemie, 4th edition, vol. 23, pp. 708 ff.

Ullmann's Encyklopädie der technischen Chemie, 4th edition, vol. 19, pp. 602 ff.

Primary Examiner—Herbert J. Lilling
Attorney, Agent, or Firm—Fisher, Christen & Sabol

[57] **ABSTRACT**

A process for preparing nicotinamide, wherein, in the first stage, 2-methyl-1,5-diaminopentane is catalytically converted into 3-picoline, then the 3-picoline is converted via an ammonoxidation into 3-cyanopyridine and, finally, the 3-cyanopyridine is converted microbiologically into the nicotinamide.

26 Claims, No Drawings

PROCESS FOR PREPARING NICOTINAMIDE

BACKGROUND OF THE INVENTION

1. Field of the Invention

The invention relates to a new process for preparing nicotinamide.

2. Background Art

Numerous processes are known for the preparation of nicotinamide, which is one of the B-group vitamins essential to man and beast. Essentially only two processes have achieved industrial importance, namely, the nitric acid oxidation of alkylpyridines and the ammonoxidation of alkylpyridines (cf. *Ullmann's Encyklopädie der technischen Chemie,* 4th edition, Vol. 23, pp. 708 ff. and Vol. 19, pp. 602 ff.).

Although the nitric acid oxidation, specifically of 2-methyl-5-ethylpyridine, is a very selective process, it incorporates a risk potential for the minimization of which highly qualified personnel, optimum infrastructure and a high standard of know-how are indispensable prerequisites. Such process of nitric acid oxidation is, therefore, unsuitable for technology transfer, for example to places where the prerequisites mentioned can only be realized in part.

The ammonoxidation, specifically of 3-picoline, has not previously come close to the industrial importance of the nitric acid oxidation, although numerous publications describe quantitative conversions with yields of over 90 percent (cf. *Ullmann's Encyklopädie der technischen Chemie,* 4th Edition, Vol. 19, pp. 602 ff.). Essential prerequisites for an industrially usable catalyst are not only its degree of conversion and its selectivity, but likewise are the achievable space velocity over the catalyst (amount of starting material/catalyst volume/time=kg $l^{-1}h^{-1}$) and its operating life. Particularly in respect of the last two criteria, the known ammonoxidation catalysts from the prior art are not satisfactory.

BROAD DESCRIPTION OF THE INVENTION

An object of the invention is to provide an industrially usable process which, on the one hand, is based on a technology which is relatively simple to master and, on the other hand, meets all of the criteria and requirements of an economical process. Other objects and advantages of the invention are set out herein or are obvious herefrom to one skilled in the art.

The objects and advantages of the invention are achieved by the process of the invention.

According to the process of the invention for preparing nicotinamide, In the first stage:

(a) 2-methyl-1,5-diaminopentane in the gas phase at 300° to 400° C. and at 0 to 10 bar gauge pressure is converted into 3-methylpiperidine by passing it over a catalyst containing as the active component at least one oxide of Al and/or Si, having at the surface a ratio of acid centers to basic centers of more than 2 and having a specific surface area of more than 40 m^2/g, and, immediately afterwards, the 3-methylpiperidine is passed at 220° to 400° C. over a dehydrogenation catalyst and is converted into 3-picoline, then in the second stage:

(b) 3-picoline is, in the presence of ammonia and an oxygen-containing gas, passed at 280° to 400° C. over an ammonoxidation catalyst comprising the oxides of vanadium, titanium, zirconium and molybdenum in a molar ratio of V_2O_5 to TiO_2 to ZrO_2 of from 1:1:2, respectively, to 1:12:25, respectively, and having an MoO_3 content, based on the V_2O_5, of from 0.54 percent by weight to 2.6 percent by weight,

and, finally, in the third stage:

(c) the resultant 3-cyanopyridine is converted by means of microorganisms of the genus Rhodococcus into the end product.

DETAILED DESCRIPTION OF THE INVENTION

The first process stage, viz. the preparation of 3-picoline from 2-methyl-1,5-diaminopentane, is comprehensively described in (a) PCT Published Application WO 94/22824, and (b) U.S. patent application Ser. No. 08/525,744.

U.S. patent application Ser. No. 08/525,744, applicants: Josef Heveling, et al., entitled: "Process For The Preparation Of 3-Methylpiperidine and 3-Methylpiperidine and 3-Methyl Pyridine by catalytic cyclization of 2-methyl-1,5-Diaminopentane", filed on Oct. 2, 1995, is commonly owned with this application. The pertinent portions of U.S. patent application Ser. No. 08/525,744 are incorporated herein by reference.

U.S. patent application Ser. No. 08/525,744 discloses a process for the preparation of 3-methylpyridine (that is, 3-picoline), wherein, first, 3-methylpiperidine is prepared from 2-methyl-1,5-diaminopentane in the gas phase at 300° to 400° C. and at 0 to 10 bar above atmospheric by passing the starting material over a catalyst which contains, as the active component, at least one oxide of Al and/or Si, which has a ratio between acid and basic centers on the surface of greater than 2 and has a specific surface area of greater than 40 m^2/g, and the resultant 3-methylpiperidine is subsequently passed over a dehydrogenation catalyst, preferably at 220° to 400° C. The dehydrogenation catalyst used is a noble metal, such as, palladium or platinum, on a support. The dehydrogenation catalyst preferably is palladium on an amorphous silicon/aluminum oxide which has been prepared by ion exchange with a soluble palladium complex.

The term "oxides of Al and/or Si" is taken to mean the individual oxides, such as Al_2O_3, mixed oxides of Al_2O_3/SiO_2 and crystallized compounds thereof, such as aluminum silicates, in particular zeolites. It is important that they have a predominantly acidic character and a specific surface area of greater than 40 m^2g. The acidic character arises from the ratio between acidic and basic centers on the surface, which must, in accordance with the invention, be greater than 2. The acidic centers are determined analytically by irreversible adsorption of NH_3 at 80° C., and the basic centers by irreversible adsorption of CO_2 at 80° C. Preferred catalysts for the novel process are activated Al_2O_3, mixed oxides of Al_2O_3/SiO_2, or zeolites. Zeolites are crystalline natural or synthetic aluminum silicates which have a highly ordered structure with a rigid three-dimensional network of SiO_4 and AlO_4 tetrahedra connected by common oxygen atoms. The ratio between the number of Si and Al atoms and oxygen is 1:2. The electrovalence of the aluminum-containing tetrahedra is compensated by inclusion of cations in the crystal, for example, alkali metal or hydrogen ions. Cation exchange is possible. The spaces between the tetrahedra are occupied by water molecules before dehydration by drying or calcination.

If the zeolite, owing to its preparation method, is not in the catalytically active, acidic H form, but instead, for example, in the Na form, it can be converted fully or partially into the desired H form by ion exchange, for example with ammonium ions, followed by calcination or by treatment with acids.

The catalysts are preferably employed as fixed-bed catalysts, and the starting material is expediently passed through the catalyst using hydrogen or an inert gas, such as nitrogen, as carrier gas.

The reaction temperature is set at 300° to 400° C., preferably at 305° to 375° C. The pressure is 0 to 10 bar, preferably 0 to 5 bar, above atmospheric.

A measure of the flow rate over catalysts is the mass hourly space velocity (MHSV). In the present case, an MHSV of 2.1 to 4.2 g of starting material per g of catalyst and per hour is advantageously maintained. The vapor-form starting material can be diluted, preferably with N_2 or H_2.

3-Methylpiperidine can be converted into 3-picoline by known dehydrogenation processes. The 3-methylpiperidine stream produced by the process of the invention can be passed directly over a dehydrogenation catalyst, so that the dehydrogenation takes place immediately after the cyclization. This is possible because the 3-methylpiperidine is produced in unusually high purity and in particular now contains virtually no MPDA, which has been found greatly to impair the activity of dehydrogenation catalysts.

The dehydrogenation catalysts used are preferably noble metals, such as, for example, Pd or Pt, on a support. Particularly advantageous dehydrogenation catalysts have been found to be those obtainable from amorphous silicon aluminum oxides by ion exchange with soluble palladium complexes, such as $[Pd(NH_3)_4]Cl_2$. The amorphous silicon aluminum oxides are advantageously first dewatered and charged with ammonia. The ion exchange with the soluble palladium complex can take place by suspension of the amorphous oxide in a solution of the complex. Alternatively, a solution of the complex can be passed through a packing of the amorphous oxide, but, in contrast to the former method, uniform loading can only be achieved by complete exchange.

The above methods also allow palladium contents of up to 5 percent by weight or more to be achieved in one step using relatively dilute solutions, for example, 0.01 mol/l of $[Pd(NH_3)_4]Cl_2$.

The reaction temperature during the dehydrogenation is preferably 220° to 400° C. In one embodiment, the cyclization catalyst is applied directly to the dehydrogenation catalyst bed, and the 2-methyl-1,5-diaminopentane is passed in from above. In a preferred embodiment, the catalysts are introduced into separate reactors. This allows independent temperature control and, if desired, independent catalyst regeneration.

The 3-picoline obtained can, without intermediate purification, be fed directly to the ammonoxidation stage. However, it is preferably subjected to, for example, an intermediate purification by distillation, which has a positive effect on the catalyst life in the next (second) stage.

The ammonoxidation in the second stage is the subject-matter of (a) PCT Published Application WO 95/32055 (PCT/EP 95/0 1945) and (b) U.S. patent application Ser. No. 08/732,343. U.S. patent application Ser. No 08/732,343, applicants: SEMBAEV et at., entitled: "Catalytic Composition For The Oxidative Ammonolysis Of Alkylpyridines", filed on the same date as this application, is commonly owned with this application. The pertinent portions of U.S. patent application Ser. No. 08/732,343 are incorporated herein by reference.

U.S. patent application Ser. No. 08/732,343 discloses a catalyst composition of the oxides of vanadium, titanium, zirconium and molybdenum, for use in the oxidative ammonolysis of alkylpyridines, for example, 3-methylpyridine to the corresponding 3-cyanopyridine.

As the ammonoxidation catalyst, preference is given to using a catalyst composition comprising the oxides of vanadium, titanium, zirconium and molybdenum in a molar ratio of V_2O_5 to TiO_2 to ZrO_2 of from 1:3:4, respectively, to 1:8:16, respectively, and having a MoO_3 content, based on V_2O_5, of from 0.54 percent by weight to 1.20 percent by weight. The preparation of the catalyst is comprehensively described in the above-mentioned PCT application PCT/EP 95/01945.

As the oxygen-containing gas, preference is given to using air since air has the advantage that the oxygen is already diluted with inert gases. However, the partial pressure of oxygen can be further regulated by mixing in inert gas such as nitrogen or oxygen-free process gases obtained by recycling.

The reactants 3-picoline, ammonia and oxygen-containing gas (calculated as O_2) are advantageously passed in gas form and in a molar ratio of from 1:1:1.5, respectively, to 1:8.5:60, respectively, at 280° to 400° C., preferably 310° to 380° C., over the catalyst. The preferred molar composition of the feed gas is 3-picoline, ammonia and oxygen-containing gas (calculated as O_2) in a ratio of from 1:1:1.5, respectively, to 1:4:25, respectively.

Water can have a favorable influence on the activity of the catalyst and is advantageously passed over the catalyst in a molar ratio of water to 3-picoline of up to, and including, 5:1, respectively, and preferably about 1.5:1, respectively.

In this second stage, yields of 3-cyanopyridine of up to 99 percent are achieved at a space velocity over the catalyst of from 50 to 150 ($gl\text{-}^{-1}h^{-1}$) of 3-picoline. The catalyst life is likewise extraordinarily high and is at least one year.

As compared with the prior art, the present ammonoxidation process, as a constituent part of the process of the invention, made it possible to develop a process which satisfies all of the criteria of an industrial reaction.

The resultant 3-cyanopyridine can be fed to the biohydrolysis in the form of an aqueous solution, either directly or after a work-up step, e.g., a crystallization, extraction or distillation. A preferred work-up comprises countercurrent extraction of the 3-cyanopyridine with toluene, for example, and subsequent vacuum distillation. The solvent used, e.g., toluene, can be completely recycled.

The biohydrolysis of 3-cyanopyridine as substrate to give nicotinamide is advantageously carried out using microorganisms of the species *Rhodococcas rhodochrous, Rhodococcus sp.* S - 6 or *Rhodococas equi*, preferably using microorganisms of the species *Rhodococcus sp.* S - 6 (FERM BP-687), *Rhodococas rhodochrous J*1 (FERM BP-1478) or *Rhodococcus equi* TG328 (FERM BP-3791). In particular, the reaction is carried out by means of microorganisms of the species *Rhodococcus rhodochrous* (FERM BP-1478). The three species mentioned above were deposited by Nitto Chemical Industry Co., Ltd. in the Fermentation Research Institute, Agency of Industrial Science & Technology, Ministry of International Trade and Industry, Japan, according to the rules of the Budapest Treaty. The FERM BP-numbers are the official deposit numbers. The microorganisms of the species *Rhodococcus sp.* S - 6, *Rhoclococcus rhodochrous J*1 and *Rhodococcus equi* TG328 are microorganisms described in the literature. *Rhodocoous rhodochrous J*1(FERM BP-1478) is comprehensively described in (a) European Published Patent Application No. B 307,926, and (b) U.S. Pat. No. 5,334,519, *Rhodococcus sp.* S - 6 (FERM BP-687) in (a) European Published Patent Application No. A 0,188,316 and (b) U.S. Pat. No. 5,179,014, and and *Rhodococcus equi* TG328 (FERM BP-379 1) in U.S. Pat. No. 5,258,305.

The pertinent portions of U.S. Pat. No. 5,179,014 are incorporated herein by reference. U.S. Pat. No. 5,179,014 discloses and described *Rhodococcus sp.* S - 6, and its morphology, growth state in various culture media (30° C.), physiological characteristics and chemical composition of cells.

The pertinent portions of U.S. Pat. No. 5,334,519 are incorporated herein by reference. U.S. Pat. No. 5,334,519 discloses and describes *Rhodococcus rhodochrous sp.* J - 1, and its morphology.

The pertinent portions of U.S. Pat. No. 5,258,305 are incorporated herein by reference. U.S. Pat. No. 5,258,305 discloses and describes *Rhodococcus equi* TG328, and its morphology, growth on culture media (at 30° C.) and physiological properties.

Likewise suitable for the process are the functionally equivalent variants and routants of these microorganisms. For the purposes of the present invention, "functionally equivalent variants and mutants" are microorganisms which have essentially the same properties and functions as the original microorganisms. Such variants and mutants can arise by chance, for example, by means of UV irradiation.

The microorganisms are usually cultured (grown) and the effective enzymes induced prior to the actual biotransformation as described in European Published Patent Application No. B 307,928. The biotransformation is preferably carried out using, as is customary in the art, immobilized microorganism cells.

The biotransformation is advantageously carried out in a pH range of from 6 to 10, preferably in a pH range of from 6.5 to 8.5. The pH is here advantageously set using a suitable phosphate buffer.

The biotransformation can be carried out at a temperature of from 5° to 50° C., preferably from 15° to 30° C.

Preferably, the biohydrolysis of the 3-cyanopyridine, which is advantageously present in aqueous solution in a concentration of from 5 to 30 percent by weight, is carried out in a reactor cascade comprising from 2 to 5 connected stirred reactors which each contain the biocatalyst. Particular preference is given to using cascades comprising 3 or 4 stirred vessels. The 3-cyanaopyridine content of the aqueous solution particularly preferably fluctuates between 10 and 20 percent by weight.

After a residence time of from 5 to 30 hours, the nicotinamide can be isolated from the product stream, for example, by crystallization. Preferably, the reaction solution is purified over activated carbon or a polystyrene resin (e.g., Amberlite) and the nicotinamide is isolated from the aqueous phase in a conventional manner.

The conversion in the biohydrolysis is virtually quantitative and gives a nicotinamide having a purity of over 99.5 percent.

The most preferred embodiments of the invention are set out in the following examples.

EXAMPLE 1a

MPDA (methytdiaminopentane) to 3-picoline

A reactor (13 mm ϕ) was charged with 4 g of a Pd catalyst (1% Pd/Al_2O_3) and, on top of that, 3 g of H-ZSM-5 [54.5% of pentasil (Si/Al=18) plus 45.5% of binder]. (The starting material was always fed into the reactor from the top.) The reaction conditions were: temperature: 305° to 320° C., 15 ml/min of N_2, and pressure: 5 bar. In a temperature range of 305° to 320° C. and at an MHSV (mass hourly space velocity over the catalyst) of 0.6 g/ (g·h), yields of up to 97 percent of 3-picoline were achieved, with the only further product found being 2.9 percent of MPI (methylpiperadine). Thus, complete conversion of the MPDA to desired products took place. No deactivation of the catalysts were observed over a period of 10 days. H_2 can be used as the carrier gas in place of N_2.

EXAMPLE 1b

Preparation of 3-picoline Using Two Separate Reactors and Commercial MPDA (MPDA to 3-picoline in 2 Stages With Isolation of MPI)

1st Stage: A reactor (13 mm ϕ) was charged with 3 g of ZSM-5 in the ammonium form (particle size: 0.5 to 1 mm). MPDA was vaporized and, together with a carrier gas stream of 15 ml/minute of N_2, was passed at a pressure of 5 bar and a temperature of 335° C. over the catalyst. The MHSV was 4.2 g of MPDA per gram of catalyst per hour. The MPDA used was a commercial product obtainable from DuPont de Nemours under the trade name Dytek A. The experiment ran for 280 hours. A deactivation of the catalyst was not observed. The product was condensed and the ammonia formed was able to escape. The yields of MPI were virtually quantitative (>99.5 percent).

2nd Stage: A reactor (13 mm ϕ) was charged with 10 g of a Pd-$MgCl_2$,Al_2O_3 dehydrogenation catalyst. The MPI from the first stage was passed in vapor form together with a carrier gas stream of 15 ml/minute of N_2 at a pressure of 1 bar and a temperature of 280° C. over the catalyst. The MHSV was 0.23 g of MPI per gram of catalyst per hour. The experiment ran for 190 hours. A deactivation of the catalyst was not observed. After 190 hours, the following product composition was determined by gas chromatography: 99.3 percent of 3-picoline, and 0.4 percent of MPI.

EXAMPLE 1c

Preparation of 3-picoline Using Two Separate Reactors and Commercial MPDA (MPDA to 3-picoline in 2 Stages Without Isolation of MPI)

A reactor (13 mm ϕ) was charged with 3 g of NH_4-ZSM-5 (particle size: 0.5 to 1 mm). MPDA was vaporized and, together with a carrier gas stream of 15 ml/minute of N_2, passed at a pressure of about 1 bar and a temperature of 320° C. over the catalyst. The MHSV was between 1 and 2 g of MPDA per gram of ZSM-5 per hour. The MPDA used was a commercial product obtainable from DuPont de Nemours under the trade name Dytek A. The product from the cyclization reactor was kept in the gas phase and conveyed directly to a second reactor. This reactor contained 12 g of a alehydrogenation catalyst composed of Pd and $MgCl_2$ on an Al_2O_3 support (particle size: 0.32 to 1 mm). The reaction conditions were 280° C. and about 1 bar. The condensate from the dehydrogenation reactor contained, after a reaction time of 220 hours, 99.1 percent of 3-picoline and 0.9 percent of MPI (by gas chromatography). A deactivation of the two catalysts over the reaction time was not observed.

EXAMPLE 1d

2-Methyl-1,5-daiminopentane (MPDA) to 3-picoline Continuously in Two Stages

A reactor (13 mm ϕ) was charged with 3 g of SiO_2,Al_2O_3 granules (Si-HP-87-069 T from Engelhard) having a particle size of 0.315 to 1 mm. MPDA was vaporized and, together with a carrier gas stream of 15 ml/minute of H_2, passed at a pressure of about 1 bar and a reactor temperature of 320° C. over the catalyst and cyclized to form MPI. The MPDA used was a commercial product obtainable from DuPont de Nemours under the trade name Dytek A. The product from the cyclization reactor was kept in the gas phase and conveyed directly to a second reactor. This reactor contained 3 g of the dehydrogenation catalyst from Example 18 of WO 94/22824 (particle size: 0.32 to 1 mm). The reactor temperature was 280° C., the pressure was 1 bar. During the course of the experiment, the starting material MPDA was converted into MPI and then into a crude product (3-MP crude) consisting of a mixture having the following composition: 74.9 percent of MPI, 13.9 percent of MPDA, 5.1 percent of organic impurities (mainly methylcyclopentanediamines) and 6.1 percent of water. The results together with the associated MHSVs (MHSV based on Reactor 1) are shown in the following table:

Starting	MHSV	GC % by area		Running Time	Deacti-vation
Material	[l/h]	PIC	MPI	[h]	[PIC %/h]
Dytek A	2.1	99.7	—	71	0
Dytek A	3.15	99.6	0.2	25	0
Dytek A	4.2	98.6	1.4	48	0
MPI	4.1	95.2	3.8	3	—
MPI	3.52	98.6	0.6	92	0
3-MP crude	4.2	93.9	1.5	170	0.0172

EXAMPLE 2a

Ammonoxidation of 3-picoline to 3-cyanopyridine

36.4 g of vanadium pentoxide, 48.0 g of titanium dioxide, 197.2 g of zirconium dioxide and 0.42 g of molybdenum trioxide were milled in a ball mill. The molar ratio of V_2O_5:TiO_2:ZrO_2 was 1:3:8, respectively, and the MoO_3 content was 1.15 percent by weight, based on V_2O_5. Pellets having dimensions of 5×5 mm were formed from the mixture. These were subjected to a heat treatment (100° to 120° C., for 6 hours in a stream of air). 60 cm^3 (82 g) of the catalyst thus pretreated were placed in a tube reactor (stainless steel, internal diameter 20 mm, length 1,000 mm). At a catalyst bed temperature of 330° C., a mixture of 3-picoline, air and ammonia was then passed over the catalyst at a feed rate of (g per 1 of catalyst per hour=$gl^{-1}h^{-1}$) 84 $gl^{-1}h^{-1}$ of 3-picoline; 2,000 $gl^{-1}h^{-1}$ of air; and 9.92 $gl^{-1}h^{-1}$ of ammonia. The molar composition of the feed gas was 3-picoline:O_2:NH_3=1:40:1.3. Accordingly, 25.5 g of 3-picoline was passed over the catalyst in 10 hours. The conversion was 100 percent. 26.8 g of 3-cyanopyridine was obtained, which corresponds to a yield of 95.0 percent.

EXAMPLE 2b

Ammonoxidation of 3-picoline to 3-cyanopyridine (in a Multitube Reactor Without Additional Thermal Treatment of the Catalyst)

11.67 kg of vanadium pentoxide, 25.12 kg of titanium oxide as metatitanic acid, 63.22 kg of zirconium oxide and 1124 g of molybdenum trioxide (as ammonium paramolybdate) were milled in a ball mill. The molar ratio of V_2O_5:TiO_2:ZrO_2 was 1:4:8, respectively, and the MoO_3 content was 1.13 percent, based on V_2O_5. Pellets having dimensions of 6×6 mm were formed from the mixture. These were subjected to a heat treatment (100° to 120° C., for 6 hours in a stream of air).

A quantity (72 kg, 53 liters) was placed in a tube reactor (stainless steel, internal diameter 21 mm, length 3,000 mm, number of tubes 51). At a catalyst bed temperature of 340° C., a mixture of 3-picoline, air, recirculated waste gas and ammonia was then passed over the catalyst at a feed rate of (g per 1 of catalyst per hour=$gl^{-1}h^{-1}$) 3.1 kgh^{-1} of 3-picoline (60 $gl^{-1}h^{-1}$), 7.6 kgh^{-1} of air, 67.0 kgh^{-1} of waste gas, and 0.84 kgh^{-1} of ammonia. The molar composition of the feed gas was 3-picoline:O_2:NH_3=1:1.9:1.5, respectively. Accordingly, 1,860 kg of 3-picoline was passed over the catalyst in 600 hours. 1,880 kg of 3-cyanopyridine was obtained, which corresponds to a yield of 90.4 percent.

EXAMPLE 2c

Ammonoxidation of 3-picoline to 3-cyanopyridine (in a Single-tube Reactor with Additional Thermal Treatment of the Catalyst)

A quantity of the catalyst obtained in Example 2b (135 cm^3, 160 g) was treated thermally at 620° C. for 6 hours in a stream of air. This was subsequently placed in a tube reactor (internal diameter 21 mm, length 1,000 mm). At a catalyst bed temperature of 375° C., a mixture of 3-picoline, air, nitrogen and ammonia was passed over the catalyst. The feed rate was 11 gh^{-1} of 3-picoline (corresponds to 81 g of picoline per liter of catalyst per hour), 30 lh^{-1} of air, 285 lh^{-1} of nitrogen, and 4 gh^{-1} of ammonia, corresponding to a molar ratio of 3-picoline:O_2:NH_3 of 1:2:2.6, respectively. After 24 hours, 264 g of picoline had been passed over the catalyst bed. The conversion was 99 percent. 261 g of 3-cyanopyridine was obtained, viz. a yield of 89 percent. The productivity of 3-cyanopyridine was 80 $gl^{-1}h^{-1}$.

EXAMPLE 2d

Ammonoxidation of 3-picoline to 3-cyanopyridine (in a Single-tube Reactor with Smaller Pellets and Higher Picoline Productivity)

Pellets having dimensions between 3 and 4 mm were formed from the catalyst obtained in Example 2b. A quantity (1 liter, 1.5 kg) was placed in a tube reactor (stainless steel, internal diameter 21 mm, length 3,000 mm). A mixture of 3-picoline, air, nitrogen and ammonia was passed over the catalyst at a catalyst bed temperature of 353° C. The feed rate was 96 gh^{-1} of 3-picoline (corresponds to 96 g of picoline per liter of catalyst per hour), 210 lh^{-1} of air, 1,340 lh^{-1} of nitrogen, and 60 gh^{-1} of ammonia. Accordingly, 2,305 g of 3-picoline were passed over the catalyst bed in 24 hours. 2,380 g of 3-cyanopyridine was obtained, which corresponds to a yield of 90 percent. The 3-picoline conversion was 97.5 percent.

Oxidative ammonolysis of picoline (3-Pic)

	Catalyst Composition				Gas feed in g/Letter of catalyst/h					3-Cyanopyridine	
	in mol			% by weight based on V_2O_5		Air or air		Temperature	Conversion	Molar	Productivity in g/l of
Example	V_2O_5	TiO_2	ZrO_2	MoO_3	3-Pic	mixture	Ammonia	°C.	%	Yield %	catalyst/h
2a	1	3	8	1.15	84	1667	9.9	330°	100	95	89.3
2b	1	4	8	1.13	60	1407	15.8	340°	100	90.4	60.7
2c	1	4	8	1.13	81	1944	29.6	375°	99	89.0	80.6
2d	1	4	8	1.13	96	1550	60.0	353°	97.5	90.0	96.6

EXAMPLE 3a

Preparation of Nicotinamide (NA) from 3-cyanopyridine

In a cascade comprising a 1.125 l reactor and two 0.375 l reactors, a 10 percent strength solution of 3-cyanopyridine was converted into NA. At a throughput rate of 300 ml/hr of stating material solution, cyanopyridine was converted quantitatively into NA; the first reactor contained 45 g of immobilized microorganisms. The biocatalyst remained in the respective reactors during the entire experiment. The biocatalyst contained immobilized microorganisms of the species *Rhodococcus rhodochrous J1*.

The reaction occurred at a temperature of 25°±1° C. and a pH of from 8 to 8.5. The pH was set using phosphoric acid and sodium hydroxide solution. In this experiment, the reaction of cyanopyridine proceeded for 2,400 hours, without the product stream containing more than 0.05 percent of cyanopyridine, which corresponds to a conversion of >99.5 percent. The activity of the catalyst was exhausted after this time.

Product solution containing from 14 to 15 percent of NA was filtered through a 0.2 μm sterilizing filter. The clear product solution obtained was subsequently evaporated to dryness. The product obtained contained >99.7 percent of NA (titration) and corresponded to pharmaceutical quality.

EXAMPLE 3b

Preparation of NA from 3-cyanopyridine

In a cascade comprising a 150 l reactor and two 45 l reactors, a 15 percent strength solution of 3-cyanopyridine was converted into NA. At a throughput rate of 25 l/h of starting material solution, cyanopyridine was quantitatively converted into NA; the first reactor contained 6 kg of immobilized microorganisms (dry weight) and the two further reactors each contained 0.9 kg (dry weight) of immobilized microorganisms. The biocatalyst remained in the respective reactors during the entire experiment. The biocatalyst contained immobilized microorganisms of the species *Rhodococcus rhodochrous J1*.

The reaction occurred at a temperature of 24°±2° C. and a pH of from 7 to 8.5. The pH was set using phosphoric acid and sodium hydroxide solution, with potassium dihydrogen phosphate also being used for buffering (1 to 3 mg/l).

In this experiment, the reaction of cyanopyridine proceeded for 1,800 hours, without the product stream containing more than 0.1 percent of cyanopyridine, which corresponds to a conversion of >99.0 percent. The activity of the biocatalyst was exhausted after this time.

Product solution containing from 18 to 20 percent of NA was subsequently purified continuously in fixed-bed adsorbers (each having a volume of 15.7 l), with from 0.5 to 4 percent of activated carbon (based on amount of product) and from 0.5 to 2 percent of Amberlite XAD2 being used.

Additionally purified NA solution was subsequently filtered continuously. Use was made of a three-stage filtration system in which the product solution was first fed to a GAF filter (10 to 30 μm pore size), subsequently to a sterilizing filter (pore size 0.2 μm) and finally to an ultrafiltration (pore size from 10,000 to 30,000 Dalton).

The filtered product solution was concentrated in a falling-film evaporator to from 60 to 80 percent of NA. Water removed from the product could be recirculated to the biohydrolysis. The product was isolated in a spray dryer having an integrated fluidized bed (fluidized spray dryer).

The product obtained contained >99.7 percent of NA (titration) and corresponded to pharmaceutical quality.

What is claimed is:

1. Process for preparing nicotinamide, comprising: in a first stage

(a) 2-methyl-1,5-diaminopentane in the gas phase at 300° to 400° C. and at 0 to 10 bar gauge pressure is converted into 3-methylpiperidine by passing it over a catalyst containing as active component at least one oxide of Al and/or Si, having at the surface a ratio of acid centers to basic centers of more than 2 and having a specific surface area of more than 40 m^2/g, and, immediately afterwards, the 3-methylpiperidine is passed at 220° to 400° C. over a dehydrogenation catalyst and is converted into 3-picoline,

then in a second stage

(b) the 3-picoline is, in the presence of ammonia and an oxygen-containing gas, passed at 280° to 400° C. over an ammonoxidation catalyst comprising the oxides of vanadium, titanium, zirconium and molybdenum in a molar ratio of V_2O_5 to TiO_2 to ZrO_2 of from 1:1:2, respectively, to 1:12:25, respectively, and having a MoO_3 content, based on V_2O_5, of from 0.54 percent by weight to 2.6 percent by weight,

and, finally, in a third stage

(c) the resultant 3-cyanopyridine is converted by means of microorganisms of the genus Rhodococcus into nicotinamide.

2. The process according to claim 1, wherein the dehydrogenation catalyst used in the first stage is a noble metal catalyst on a support.

3. The process according to claim 2, wherein the ammonoxidation catalyst used is a catalyst composition comprising

the oxides of vanadium, titanium, zirconium and molybdenum in a molar ratio of V_2O_5 to TiO_2 to ZrO_2 of from 1:3:4, respectively, to 1:8: 16, respectively, and having a MoO_3 content, based on V_2O_5, of from 0.54 percent by weight to 1.20 percent by weight.

4. The process according to claim **3**, wherein, in the second stage, 3-picoline, ammonia and the oxygen-containing gas, which is calculated as O_2, are passed in a molar ratio of from 1:1:1.5, respectively, to 1:8.5:60, respectively, at 310° to 380° C. over the catalyst.

5. The process according to claim **4**, wherein 3-picoline, ammonia and the oxygen-containing gas, which is calculated as O_2, are passed in a molar ratio of from 1:1:10, respectively, to 1:4:60, respectively, at from 310° to 380° C. over the catalyst.

6. The process according to claim **5**, wherein the microbiological reaction in the third stage is carried out using microorganisms of the species *Rhodococcus rhodochrous* or using mutants thereof.

7. The process according to claim **6**, wherein immobilized microorganisms of the species *Rhodococcus rhodochrous* are used.

8. The process according to claim **7**, wherein the microbiological reaction in the third stage is carried out at a pH of from 6 to 10 and a temperature of from 5° to 50° C.

9. The process according to claim **8**, wherein the microbiological reaction in the third stage is carried out in a reactor cascade comprising from 2 to 5 connected stirred reactors.

10. The process according to claim **1**, wherein the ammonoxidation catalyst used is a catalyst composition comprising the oxides of vanadium, titanium, zirconium and molybdenum in a molar ratio of Vhd $2O_5$ to TiO_2 to ZrO_2 of from 1:3:4, respectively, to 1:8:16, respectively, and having a MoO_3 content, based on V_2O_5, of from 0.54 percent by weight to 1.20 percent by weight.

11. The process according to claim **1**, wherein, in the second stage, 3-picoline, ammonia and the oxygen-containing gas, which is calculated as O_2, are passed in a molar ratio of from 1:1:1.5, respectively, to 1:8.5:60, respectively, at 310° to 380° C. over the catalyst.

12. The process according to claim **1**, wherein the microbiological reaction in the third stage is carried out using microorganisms of the species *Rhodococcus rhodochrous* or using mutants thereof.

13. The process according to claim **1**, wherein the microbiological reaction in the third stage is carried out at a pH of from 6 to 10 and a temperature of from 5° to 50° C.

14. The process according to claim **1**, wherein the microbiological reaction in the third stage is carried out in a reactor cascade comprising from 2 to 5 connected stirred reactors.

15. Process for preparing nicotinamide, comprising passing 3-picoline, in the presence of ammonia and an oxygen-containing gas, at 280° to 400° C. over an ammonoxidation catalyst comprising the oxides of vanadium, titanium, zirconium and molybdenum in a molar ratio of V_2O_5 to TiO_2 to ZrO_2 of from 1:1:2, respectively, to 1:12:25, respectively, and having a MoO_3 content, based on V_2O_5, of from 0.54 percent by weight to 2.6 percent by weight, and subsequently converting the resultant 3-cyanopyridine by means of microorganisms of the genus Rhodococcus into nicotinamide.

16. The process according to claim **15**, wherein the ammonoxidation catalyst used is a catalyst composition comprising the oxides of vanadium, titanium, zirconium and molybdenum in a molar ratio of V_2O_5 to TiO_2 to ZrO_2 of from 1:3:4, respectively, to 1:8:16, respectively, and having a MoO_3 content, based on V_2O_5, of from 0.54 percent by weight to 1.20 percent by weight.

17. The process according to claim **16**, wherein 3-picoline, ammonia and the oxygen-containing gas, which is calculated as O_2, are passed in a molar ratio of from 1:1:1.5, respectively, to 1:8.5:60, respectively, at 310° to 380° C. over the catalyst.

18. The process according to claim **17**, wherein 3-picoline, ammonia and the oxygen-containing gas, which is calculated as O_2, are passed in a molar ratio of from 1:1:10, respectively, to 1:4:60, respectively, over the catalyst.

19. The process according to claim **18**, wherein the microbiological reaction is carried out using microorganisms of the species *Rhodococcus rhodochrous* or using mutants thereof.

20. The process according to claim **19**, wherein immobilized microorganisms of the species *Rhodococcus rhodochrous* are used.

21. The process according to claim **20**, wherein the microbiological reaction is carried out at a pH of from 6 to 10 and a temperature of from 5° to 50° C.

22. The process according to claim **21**, wherein the microbiological reaction is carried out in a reactor cascade comprising from 2 to 5 connected stirred reactors.

23. The process according to claim **15**, wherein 3-picoline, ammonia and the oxygen-containing gas, which is calculated as O_2, are passed in a molar ratio of from 1:1:1.5, respectively, to 1:8.5:60, respectively, at 310° to 380° C. over the catalyst.

24. The process according to claim **15**, wherein the microbiological reaction is carded out using microorganisms of the species *Rhodococcus rhodochrous* or using mutants thereof.

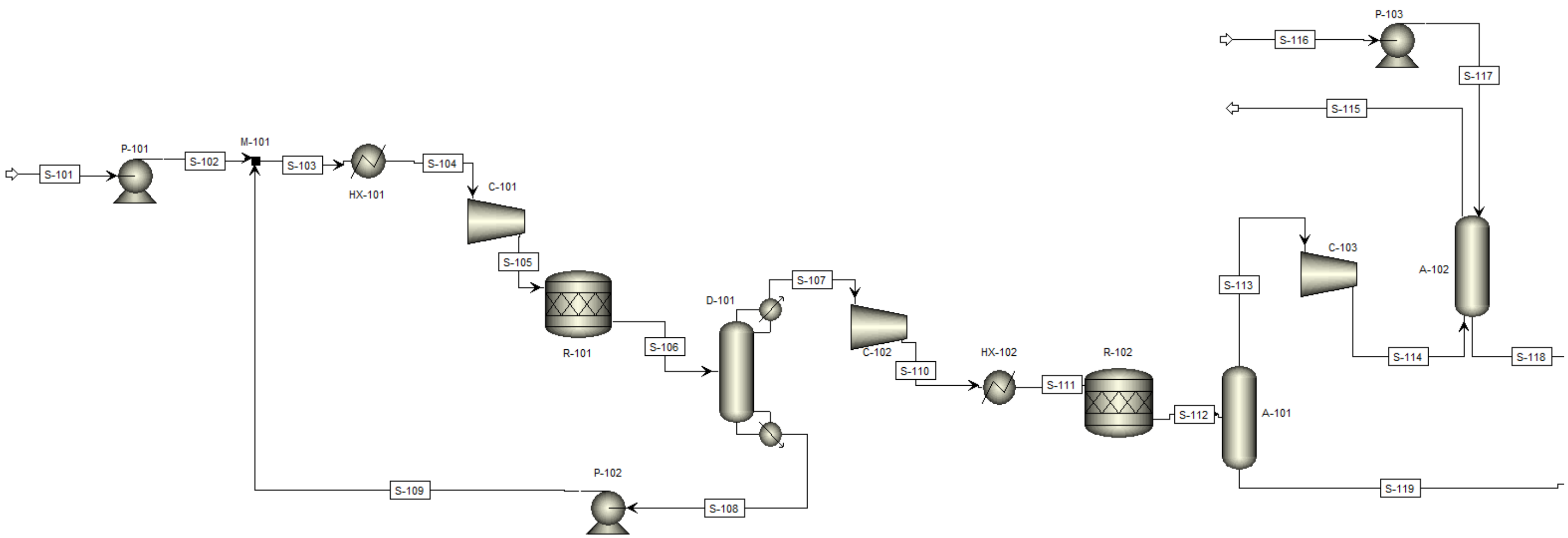
25. The process according to claim **15**, wherein the microbiological reaction is carried out at a pH of from 6 to 10 and a temperature of from 5° to 50° C.

26. The process according to claim **15**, wherein the microbiological reaction is carried out in a reactor cascade comprising from 2 to 5 connected stirred reactors.

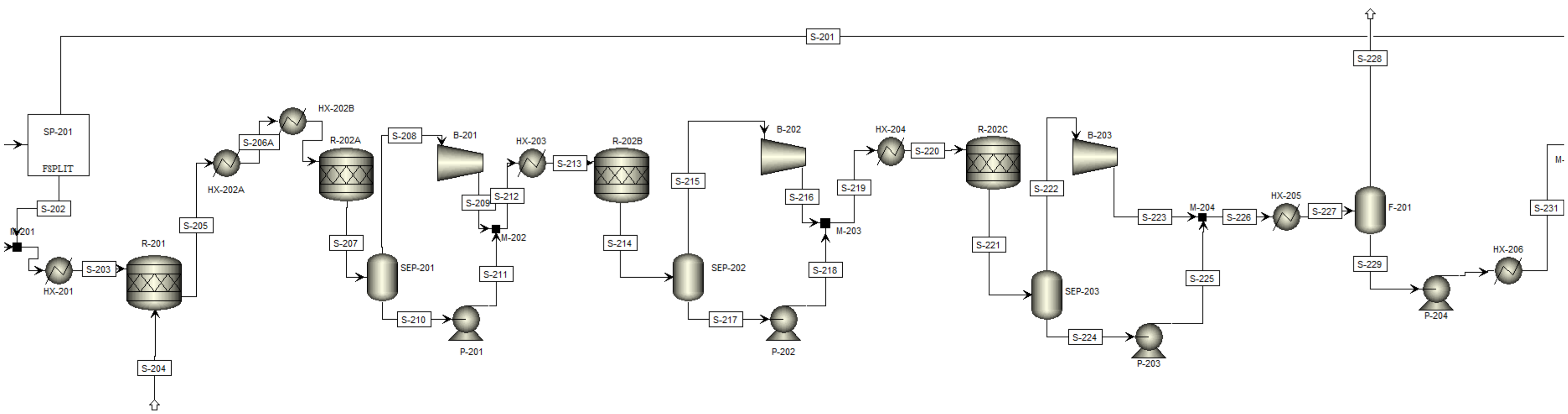
* * * * *

C. ASPEN SIMULATIONS AND REPORTS

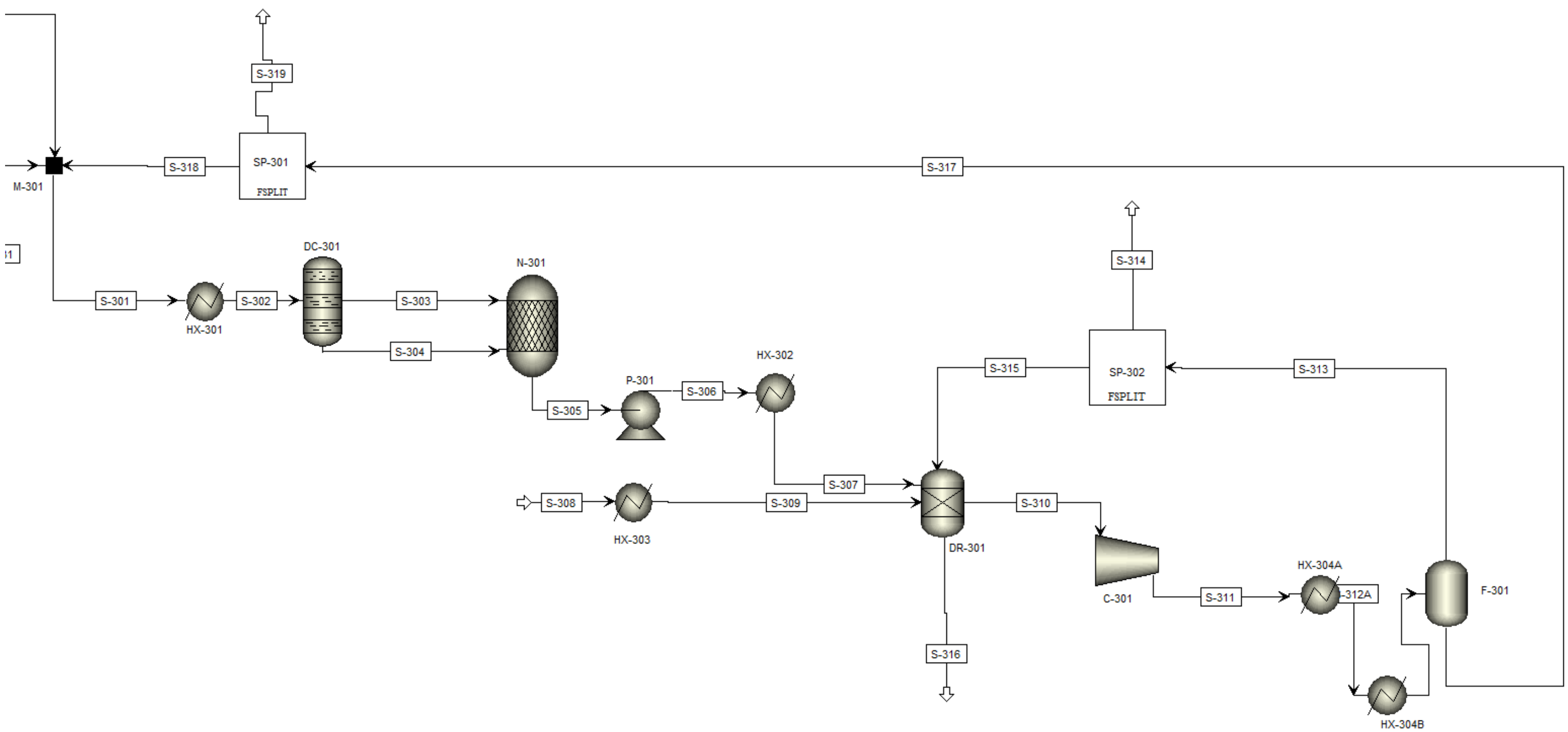
Section 100



Section 200


S-201
S-228
SP-201
FSPLIT
S-202
M-201
HX-201
S-203
R-201
S-204
S-205
HX-202A
S-206A
HX-202B
R-202A
S-207
SEP-201
S-208
B-201
S-209
S-210
P-201
S-211
M-202
S-212
HX-203
S-213
R-202B
S-214
SEP-202
S-215
B-202
S-216
S-217
P-202
S-218
M-203
S-219
HX-204
S-220
R-202C
S-221
SEP-203
S-222
B-203
S-223
S-224
P-203
S-225
M-204
S-226
HX-205
S-227
F-201
S-229
P-204
HX-206
S-231

Section 300


S-319
SP-301
FSPLIT
S-318
M-301
S-317
S-314
DC-301
N-301
S-301
HX-301
S-302
S-303
S-304
HX-302
S-315
SP-302
FSPLIT
S-313
P-301
S-306
S-305
S-307
S-308
HX-303
S-309
S-310
DR-301
C-301
HX-304A
S-311
312A
F-301
S-316
HX-304B

ASPEN Simulation Results:

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 1
NIACIN PRODUCTION
RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS COPY OF ASPEN PLUS LICENSED TO UNIVERSITY OF PENNSYLVAN

TYPE OF RUN: NEW

INPUT FILE NAME: _3810jxn.inm

OUTPUT PROBLEM DATA FILE NAME: _3810jxn
LOCATED IN:

PDF SIZE USED FOR INPUT TRANSLATION:
NUMBER OF FILE RECORDS (PSIZE) = 0
NUMBER OF IN-CORE RECORDS = 256
PSIZE NEEDED FOR SIMULATION = 256

CALLING PROGRAM NAME: apmain
LOCATED IN: C:\PROGRA~2\ASPENT~1\ASPENP~2.3\Engine\xeq

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

DESCRIPTION

General Simulation with Metric Units : C, bar, kg/hr, kmol/hr, Gcal/hr, cum/hr. Property Method: None Flow basis for input: Mole Stream report composition: Mole flow

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 2
NIACIN PRODUCTION
FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
S-204	----	R-201	S-308	----	HX-303
S-101	----	P-101	S-116	----	P-103
S-104	HX-101	C-101	S-106	R-101	D-101
S-112	R-102	A-101	S-205	R-201	HX-202A
S-207	R-202A	SEP-201	S-309	HX-303	DR-301
S-301	M-301	HX-301	S-305	N-301	P-301
S-313	F-301	SP-302	S-317	F-301	SP-301
S-310	DR-301	C-301	S-316	DR-301	----
S-315	SP-302	DR-301	S-314	SP-302	----
S-105	C-101	R-101	S-304	DC-301	N-301
S-303	DC-301	N-301	S-302	HX-301	DC-301
S-206A	HX-202A	HX-202B	S-110	C-102	HX-102
S-319	SP-301	----	S-318	SP-301	M-301
S-307	HX-302	DR-301	S-311	C-301	HX-304A
S-227	HX-205	F-201	S-102	P-101	M-101
S-312A	HX-304A	HX-304B	S-109	P-102	M-101
S-103	M-101	HX-101	S-230	P-204	HX-206
S-306	P-301	HX-302	S-111	HX-102	R-102
S-203	HX-201	R-201	S-208	SEP-201	B-201
S-210	SEP-201	P-201	S-211	P-201	M-202
S-212	M-202	HX-203	S-214	R-202B	SEP-202
S-221	R-202C	SEP-203	S-222	SEP-203	B-203
S-224	SEP-203	P-203	S-215	SEP-202	B-202
S-217	SEP-202	P-202	S-219	M-203	HX-204
S-226	M-204	HX-205	S-218	P-202	M-203
S-225	P-203	M-204	S-209	B-201	M-202
S-216	B-202	M-203	S-223	B-203	M-204
S-213	HX-203	R-202B	S-220	HX-204	R-202C
S-228	F-201	----	S-229	F-201	P-204
S-113	A-101	C-103	S-119	A-101	M-201
S-115	A-102	----	S-118	A-102	SP-201
S-114	C-103	A-102	S-202	SP-201	M-201
S-201	SP-201	M-301	S-231	HX-206	M-301
S-117	P-103	A-102	S-206	HX-202B	R-202A
S-312	HX-304B	F-301	S-107	D-101	C-102
S-108	D-101	P-102	S-203A	M-201	HX-201

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
HX-101	S-103	S-104
R-101	S-105	S-106
R-102	S-111	S-112
R-201	S-203 S-204	S-205
R-202A	S-206	S-207
HX-303	S-308	S-309
M-301	S-231 S-318 S-201	S-301
N-301	S-304 S-303	S-305
F-301	S-312	S-313 S-317
DR-301	S-309 S-315 S-307	S-310 S-316
SP-302	S-313	S-315 S-314

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 3
                             NIACIN PRODUCTION
                              FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY BLOCKS (CONTINUED)
  C-101        S-104                         S-105
  DC-301       S-302                         S-304 S-303
  HX-301       S-301                         S-302
  HX-202A      S-205                         S-206A
  C-102        S-107                         S-110
  SP-301       S-317                         S-319 S-318
  HX-302       S-306                         S-307
  C-301        S-310                         S-311
  HX-205       S-226                         S-227
  P-101        S-101                         S-102
  HX-304A      S-311                         S-312A
  P-102        S-108                         S-109
  M-101        S-102 S-109                   S-103
  P-204        S-229                         S-230
  P-301        S-305                         S-306
  HX-102       S-110                         S-111
  HX-201       S-203A                        S-203
  SEP-201      S-207                         S-208 S-210
  P-201        S-210                         S-211
  M-202        S-209 S-211                   S-212
  R-202B       S-213                         S-214
  R-202C       S-220                         S-221
  SEP-203      S-221                         S-222 S-224
  SEP-202      S-214                         S-215 S-217
  M-203        S-216 S-218                   S-219
  M-204        S-223 S-225                   S-226
  P-202        S-217                         S-218
  P-203        S-224                         S-225
  B-201        S-208                         S-209
  B-202        S-215                         S-216
  B-203        S-222                         S-223
  HX-203       S-212                         S-213
  HX-204       S-219                         S-220
  F-201        S-227                         S-228 S-229
  A-101        S-112                         S-113 S-119
  A-102        S-114 S-117                   S-115 S-118
  C-103        S-113                         S-114
  SP-201       S-118                         S-202 S-201
  HX-206       S-230                         S-231
  P-103        S-116                         S-117
  HX-202B      S-206A                        S-206
  HX-304B      S-312A                        S-312
  D-101        S-106                         S-107 S-108
  M-201        S-119 S-202                   S-203A

CONVERGENCE STATUS SUMMARY
--------------------------

  TEAR STREAM SUMMARY
  ===================

  STREAM    MAXIMUM                   MAXIMUM     VARIABLE             CONV
  ID        ERROR        TOLERANCE    ERR/TOL     ID              STAT  BLOCK
  ------    -------      ---------    --------    --------        ----  -----
  S-108     0.13483E-27  0.14781E-27  0.91223     AMMONIA MOLEFLOW #    $OLVER01
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                 03/27/2013  PAGE 4
                             NIACIN PRODUCTION
                              FLOWSHEET SECTION

CONVERGENCE STATUS SUMMARY (CONTINUED)
  S-317     0.19002E-13  0.39649E-08  0.47926E-05 AMMONIA MOLEFLOW #   $OLVER02
  S-313     0.14073E-13  0.14163E-13  0.99363     WATER MOLEFLOW   #   $OLVER02

  #  = CONVERGED
  *  = NOT CONVERGED

CONVERGENCE BLOCK:  $OLVER01
----------------------------
    Tear Stream  :  S-108
    Tolerance used:  0.100D-04
    Trace molefrac:  0.100D-06
    Trace substr-2:  0.100D-06

    MAXIT=   50 WAIT   1 ITERATIONS BEFORE ACCELERATING
    QMAX =   0.0     QMIN =  -5.0
    METHOD: WEGSTEIN      STATUS: CONVERGED
    TOTAL NUMBER OF ITERATIONS:     4

                         *** FINAL VALUES ***
```

VAR#	TEAR STREAM VAR	STREAM	SUBSTREA	COMPONEN	ATTRIBUT	ELEMENT	UNIT	VALUE	PREV VALUE	ERR/TOL
1	TOTAL MOLEFLOW	S-108	MIXED				LBMOL/HR	0.2875	0.2875	-1.1589-06
2	TOTAL MOLEFLOW	S-108	CIPSD				LBMOL/HR	0.0	0.0	0.0
3	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC1		MISSING	MISSING	0.0
4	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC2		MISSING	MISSING	0.0
5	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC3		MISSING	MISSING	0.0
6	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC4		MISSING	MISSING	0.0
7	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC5		MISSING	MISSING	0.0
8	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC6		MISSING	MISSING	0.0
9	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC7		MISSING	MISSING	0.0
10	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC8		MISSING	MISSING	0.0
11	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC9		MISSING	MISSING	0.0
12	SUBS-ATTR-VA	S-108	CIPSD		PSD	FRAC10		MISSING	MISSING	0.0
13	MOLE-FLOW	S-108	MIXED	OXYGEN			LBMOL/HR	0.0	0.0	0.0
14	MOLE-FLOW	S-108	MIXED	HYDROGEN			LBMOL/HR	0.0	0.0	0.0
15	MOLE-FLOW	S-108	MIXED	NITROGEN			LBMOL/HR	0.0	0.0	0.0
16	MOLE-FLOW	S-108	MIXED	AMMONIA			LBMOL/HR	1.1731-19	1.1731-19	-0.9122
17	MOLE-FLOW	S-108	MIXED	WATER			LBMOL/HR	0.0	0.0	0.0
18	MOLE-FLOW	S-108	MIXED	CARBO-01			LBMOL/HR	0.0	0.0	0.0
19	MOLE-FLOW	S-108	MIXED	NIACINAM			LBMOL/HR	0.0	0.0	0.0
20	MOLE-FLOW	S-108	MIXED	METDIAMI			LBMOL/HR	0.2874	0.2874	7.6523-05
21	MOLE-FLOW	S-108	MIXED	METHYLPI			LBMOL/HR	3.1607-05	3.1607-05	-0.7064
22	MOLE-FLOW	S-108	MIXED	3-MET-01			LBMOL/HR	0.0	0.0	0.0
23	MOLE-FLOW	S-108	MIXED	NICOT-01			LBMOL/HR	0.0	0.0	0.0
24	MOLE-FLOW	S-108	MIXED	AMMONICO			LBMOL/HR	0.0	0.0	0.0
25	PRESSURE	S-108	MIXED				PSIA	20.5459	20.5459	0.0
26	MASS ENTHALPY	S-108	MIXED				BTU/LB	-412.7500	-412.7500	1.7247-05
27	MOLE-FLOW	S-108	CIPSD	OXYGEN			LBMOL/HR	0.0	0.0	0.0
28	MOLE-FLOW	S-108	CIPSD	HYDROGEN			LBMOL/HR	0.0	0.0	0.0
29	MOLE-FLOW	S-108	CIPSD	NITROGEN			LBMOL/HR	0.0	0.0	0.0
30	MOLE-FLOW	S-108	CIPSD	AMMONIA			LBMOL/HR	0.0	0.0	0.0
31	MOLE-FLOW	S-108	CIPSD	WATER			LBMOL/HR	0.0	0.0	0.0
32	MOLE-FLOW	S-108	CIPSD	CARBO-01			LBMOL/HR	0.0	0.0	0.0
33	MOLE-FLOW	S-108	CIPSD	NIACINAM			LBMOL/HR	0.0	0.0	0.0

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 5
NIACIN PRODUCTION
FLOWSHEET SECTION

CONVERGENCE BLOCK: $OLVER01 (CONTINUED)

34	MOLE-FLOW	S-108	CIPSD	METDIAMI	LBMOL/HR	0.0	0.0	0.0
35	MOLE-FLOW	S-108	CIPSD	METHYLPI	LBMOL/HR	0.0	0.0	0.0
36	MOLE-FLOW	S-108	CIPSD	3-MET-01	LBMOL/HR	0.0	0.0	0.0
37	MOLE-FLOW	S-108	CIPSD	NICOT-01	LBMOL/HR	0.0	0.0	0.0
38	MOLE-FLOW	S-108	CIPSD	AMMONICO	LBMOL/HR	0.0	0.0	0.0
39	PRESSURE	S-108	CIPSD		PSIA	20.5459	20.5459	0.0
40	MASS ENTHALPY	S-108	CIPSD		BTU/LB	0.0	0.0	0.0

*** ITERATION HISTORY ***

TEAR STREAMS AND TEAR VARIABLES:

ITERATION	MAX-ERR/TOL	STREAM ID	VARIABLE	SUBSTREA	COMPONEN	ATTRIBUT	ELEMENT
1	0.1100E+08	S-108	MOLE-FLOW	MIXED	METHYLPI		
2	48.29	S-108	MOLE-FLOW	MIXED	METHYLPI		
3	-3.039	S-108	MOLE-FLOW	MIXED	METHYLPI		
4	-0.9122	S-108	MOLE-FLOW	MIXED	AMMONIA		

CONVERGENCE BLOCK: $OLVER02

Tear Stream : S-317 S-313
Tolerance used: 0.100D-04 0.100D-04
Trace molefrac: 0.100D-06 0.100D-09
Trace substr-2: 0.100D-06 0.100D-09

MAXIT= 50 WAIT 1 ITERATIONS BEFORE ACCELERATING
QMAX = 0.0 QMIN = -5.0
METHOD: WEGSTEIN STATUS: CONVERGED
TOTAL NUMBER OF ITERATIONS: 23

*** FINAL VALUES ***

VAR#	TEAR STREAM VAR	STREAM	SUBSTREA	COMPONEN	ATTRIBUT	ELEMENT	UNIT	VALUE	PREV VALUE	ERR/TOL
1	TOTAL MOLEFLOW	S-317	MIXED				LBMOL/HR	1230.6056	1230.6056	-3.2597-08
2	TOTAL MOLEFLOW	S-317	CIPSD				LBMOL/HR	0.0	0.0	0.0
3	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC1		MISSING	MISSING	0.0
4	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC2		MISSING	MISSING	0.0
5	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC3		MISSING	MISSING	0.0
6	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC4		MISSING	MISSING	0.0
7	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC5		MISSING	MISSING	0.0
8	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC6		MISSING	MISSING	0.0
9	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC7		MISSING	MISSING	0.0
10	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC8		MISSING	MISSING	0.0
11	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC9		MISSING	MISSING	0.0
12	SUBS-ATTR-VA	S-317	CIPSD		PSD	FRAC10		MISSING	MISSING	0.0
13	TOTAL MOLEFLOW	S-313	MIXED				LBMOL/HR	11.1805	11.1805	4.0035-02
14	TOTAL MOLEFLOW	S-313	CIPSD				LBMOL/HR	0.0	0.0	0.0
15	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC1		MISSING	MISSING	0.0
16	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC2		MISSING	MISSING	0.0
17	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC3		MISSING	MISSING	0.0

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 6
NIACIN PRODUCTION
FLOWSHEET SECTION

CONVERGENCE BLOCK: $OLVER02 (CONTINUED)

18	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC4		MISSING	MISSING	0.0
19	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC5		MISSING	MISSING	0.0
20	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC6		MISSING	MISSING	0.0
21	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC7		MISSING	MISSING	0.0
22	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC8		MISSING	MISSING	0.0
23	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC9		MISSING	MISSING	0.0
24	SUBS-ATTR-VA	S-313	CIPSD		PSD	FRAC10		MISSING	MISSING	0.0
25	MOLE-FLOW	S-317	MIXED	OXYGEN			LBMOL/HR	2.3426-05	2.3426-05	2.9391-07
26	MOLE-FLOW	S-317	MIXED	HYDROGEN			LBMOL/HR	0.0	0.0	0.0
27	MOLE-FLOW	S-317	MIXED	NITROGEN			LBMOL/HR	8.0927-05	8.0927-05	5.1445-07
28	MOLE-FLOW	S-317	MIXED	AMMONIA			LBMOL/HR	3.1468	3.1468	4.7926-06
29	MOLE-FLOW	S-317	MIXED	WATER			LBMOL/HR	1227.4582	1227.4582	-4.4974-08
30	MOLE-FLOW	S-317	MIXED	CARBO-01			LBMOL/HR	4.8173-04	4.8173-04	2.6491-07
31	MOLE-FLOW	S-317	MIXED	NIACINAM			LBMOL/HR	0.0	0.0	0.0
32	MOLE-FLOW	S-317	MIXED	METDIAMI			LBMOL/HR	0.0	0.0	0.0
33	MOLE-FLOW	S-317	MIXED	METHYLPI			LBMOL/HR	0.0	0.0	0.0
34	MOLE-FLOW	S-317	MIXED	3-MET-01			LBMOL/HR	0.0	0.0	0.0
35	MOLE-FLOW	S-317	MIXED	NICOT-01			LBMOL/HR	0.0	0.0	0.0
36	MOLE-FLOW	S-317	MIXED	AMMONICO			LBMOL/HR	0.0	0.0	0.0
37	PRESSURE	S-317	MIXED				PSIA	58.0082	58.0082	0.0
38	MASS ENTHALPY	S-317	MIXED				BTU/LB	-6938.0891	-6938.0891	5.5965-08
39	MOLE-FLOW	S-317	CIPSD	OXYGEN			LBMOL/HR	0.0	0.0	0.0
40	MOLE-FLOW	S-317	CIPSD	HYDROGEN			LBMOL/HR	0.0	0.0	0.0
41	MOLE-FLOW	S-317	CIPSD	NITROGEN			LBMOL/HR	0.0	0.0	0.0
42	MOLE-FLOW	S-317	CIPSD	AMMONIA			LBMOL/HR	0.0	0.0	0.0
43	MOLE-FLOW	S-317	CIPSD	WATER			LBMOL/HR	0.0	0.0	0.0
44	MOLE-FLOW	S-317	CIPSD	CARBO-01			LBMOL/HR	0.0	0.0	0.0
45	MOLE-FLOW	S-317	CIPSD	NIACINAM			LBMOL/HR	0.0	0.0	0.0
46	MOLE-FLOW	S-317	CIPSD	METDIAMI			LBMOL/HR	0.0	0.0	0.0
47	MOLE-FLOW	S-317	CIPSD	METHYLPI			LBMOL/HR	0.0	0.0	0.0
48	MOLE-FLOW	S-317	CIPSD	3-MET-01			LBMOL/HR	0.0	0.0	0.0
49	MOLE-FLOW	S-317	CIPSD	NICOT-01			LBMOL/HR	0.0	0.0	0.0
50	MOLE-FLOW	S-317	CIPSD	AMMONICO			LBMOL/HR	0.0	0.0	0.0
51	PRESSURE	S-317	CIPSD				PSIA	58.0082	58.0082	0.0
52	MASS ENTHALPY	S-317	CIPSD				BTU/LB	0.0	0.0	0.0
53	MOLE-FLOW	S-313	MIXED	OXYGEN			LBMOL/HR	6.6297-02	6.6297-02	4.1027-02
54	MOLE-FLOW	S-313	MIXED	HYDROGEN			LBMOL/HR	0.0	0.0	0.0
55	MOLE-FLOW	S-313	MIXED	NITROGEN			LBMOL/HR	11.0231	11.0231	4.1025-02
56	MOLE-FLOW	S-313	MIXED	AMMONIA			LBMOL/HR	1.6058-03	1.6058-03	0.3913
57	MOLE-FLOW	S-313	MIXED	WATER			LBMOL/HR	1.1241-02	1.1241-02	-0.9936
58	MOLE-FLOW	S-313	MIXED	CARBO-01			LBMOL/HR	7.8320-02	7.8320-02	4.1041-02
59	MOLE-FLOW	S-313	MIXED	NIACINAM			LBMOL/HR	0.0	0.0	0.0
60	MOLE-FLOW	S-313	MIXED	METDIAMI			LBMOL/HR	0.0	0.0	0.0
61	MOLE-FLOW	S-313	MIXED	METHYLPI			LBMOL/HR	0.0	0.0	0.0
62	MOLE-FLOW	S-313	MIXED	3-MET-01			LBMOL/HR	0.0	0.0	0.0
63	MOLE-FLOW	S-313	MIXED	NICOT-01			LBMOL/HR	0.0	0.0	0.0
64	MOLE-FLOW	S-313	MIXED	AMMONICO			LBMOL/HR	0.0	0.0	0.0
65	PRESSURE	S-313	MIXED				PSIA	58.0082	58.0082	0.0
66	MASS ENTHALPY	S-313	MIXED				BTU/LB	-57.5604	-57.5604	-9.4503-05
67	MOLE-FLOW	S-313	CIPSD	OXYGEN			LBMOL/HR	0.0	0.0	0.0
68	MOLE-FLOW	S-313	CIPSD	HYDROGEN			LBMOL/HR	0.0	0.0	0.0
69	MOLE-FLOW	S-313	CIPSD	NITROGEN			LBMOL/HR	0.0	0.0	0.0
70	MOLE-FLOW	S-313	CIPSD	AMMONIA			LBMOL/HR	0.0	0.0	0.0
71	MOLE-FLOW	S-313	CIPSD	WATER			LBMOL/HR	0.0	0.0	0.0
72	MOLE-FLOW	S-313	CIPSD	CARBO-01			LBMOL/HR	0.0	0.0	0.0

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                 03/27/2013  PAGE 7
                             NIACIN PRODUCTION
                              FLOWSHEET SECTION

CONVERGENCE BLOCK:  $OLVER02 (CONTINUED)
 73  MOLE-FLOW       S-313    CIPSD    NIACINAM                LBMOL/HR        0.0            0.0            0.0
 74  MOLE-FLOW       S-313    CIPSD    METDIAMI                LBMOL/HR        0.0            0.0            0.0
 75  MOLE-FLOW       S-313    CIPSD    METHYLPI                LBMOL/HR        0.0            0.0            0.0
 76  MOLE-FLOW       S-313    CIPSD    3-MET-01                LBMOL/HR        0.0            0.0            0.0
 77  MOLE-FLOW       S-313    CIPSD    NICOT-01                LBMOL/HR        0.0            0.0            0.0
 78  MOLE-FLOW       S-313    CIPSD    AMMONICO                LBMOL/HR        0.0            0.0            0.0
 79  PRESSURE        S-313    CIPSD                            PSIA           58.0082        58.0082         0.0
 80  MASS ENTHALPY   S-313    CIPSD                            BTU/LB          0.0            0.0            0.0

                         *** ITERATION HISTORY ***

    TEAR STREAMS AND TEAR VARIABLES:

    ITERATION   MAX-ERR/TOL   STREAM ID      VARIABLE         SUBSTREA COMPONEN ATTRIBUT ELEMENT
    ---------   -----------   ---------      ---------------- -------- -------- -------- -------
        1       0.1000E+09    S-313          SUBS-ATTR-VA     CIPSD             PSD      FRAC1
        2       0.9000E+08    S-313          MOLE-FLOW        MIXED    OXYGEN
        3       0.5625E+07    S-313          MOLE-FLOW        MIXED    WATER
        4       0.1702E+07    S-313          MOLE-FLOW        MIXED    AMMONIA
        5       0.6113E+06    S-313          MOLE-FLOW        MIXED    NITROGEN
        6       0.6743E+06    S-313          MOLE-FLOW        MIXED    AMMONIA
        7       0.1268E+07    S-313          MOLE-FLOW        MIXED    AMMONIA
        8       0.5034E+06    S-313          MOLE-FLOW        MIXED    AMMONIA
        9       0.2000E+06    S-313          MOLE-FLOW        MIXED    WATER
       10       0.1221E+06    S-313          MOLE-FLOW        MIXED    AMMONIA
       11       0.3252E+05    S-313          MOLE-FLOW        MIXED    AMMONIA
       12       0.1959E+05    S-313          MOLE-FLOW        MIXED    WATER
       13        5268.        S-313          MOLE-FLOW        MIXED    WATER
       14        2295.        S-313          MOLE-FLOW        MIXED    AMMONIA
       15       -1224.        S-313          MOLE-FLOW        MIXED    AMMONIA
       16        702.0        S-313          MOLE-FLOW        MIXED    AMMONIA
       17        147.4        S-313          MOLE-FLOW        MIXED    AMMONIA
       18        91.00        S-313          MOLE-FLOW        MIXED    WATER
       19        21.63        S-313          MOLE-FLOW        MIXED    WATER
       20       -43.42        S-313          MOLE-FLOW        MIXED    AMMONIA
       21        11.37        S-313          MOLE-FLOW        MIXED    AMMONIA
       22        1.487        S-313          MOLE-FLOW        MIXED    AMMONIA
       23      -0.9936        S-313          MOLE-FLOW        MIXED    WATER
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                 03/27/2013  PAGE 8
                            NIACIN PRODUCTION
                             FLOWSHEET SECTION

COMPUTATIONAL SEQUENCE
----------------------

SEQUENCE USED WAS:
   P-103 P-101 HX-303
   $OLVER01 P-102 M-101 HX-101 C-101 R-101 D-101
   (RETURN $OLVER01)
   C-102 HX-102 R-102 A-101 C-103 A-102 SP-201 M-201 HX-201 R-201 HX-202A
   HX-202B R-202A SEP-201 B-201 P-201 M-202 HX-203 R-202B SEP-202 B-202
   P-202 M-203 HX-204 R-202C SEP-203 B-203 P-203 M-204 HX-205 F-201 P-204
   HX-206
   $OLVER02 SP-302 SP-301 M-301 HX-301 DC-301 N-301 P-301 HX-302 DR-301
   |  C-301 HX-304A HX-304B F-301
   (RETURN $OLVER02)

OVERALL FLOWSHEET BALANCE
-------------------------

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   CONVENTIONAL COMPONENTS (LBMOL/HR)
      OXYGEN                   46.2971         4.24004       0.908417
      HYDROGEN                 0.00000         84.5231       -1.00000
      NITROGEN                 1.10231         1.11640      -0.126183E-01
      AMMONIA                  0.00000        0.566499       -1.00000
      WATER                    66.6101         122.773      -0.457451
      CARBO-01                 0.00000        0.169045       -1.00000
      NIACINAM                 0.00000         27.6135       -1.00000
      METDIAMI                 28.4590        0.311977E-04   0.999999
      METHYLPI                 0.00000        0.284590       -1.00000
      3-MET-01                 0.00000        0.253735       -1.00000
      NICOT-01                 0.00000        0.278925       -1.00000
      AMMONICO                 0.00000         0.00000        0.00000
   TOTAL BALANCE
      MOLE(LBMOL/HR)           142.468         241.818      -0.410845
      MASS(LB/HR   )           6019.26         6019.27      -0.634129E-06
      ENTHALPY(BTU/HR  )     -0.102940E+08   -0.167061E+08   0.383822

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.00000      LB/HR
   PRODUCT STREAMS CO2E         7.43964      LB/HR
   NET STREAMS CO2E PRODUCTION  7.43964      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        7.43964      LB/HR
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                 03/27/2013  PAGE 9
                             NIACIN PRODUCTION
                         PHYSICAL PROPERTIES SECTION

COMPONENTS
----------

 ID        TYPE  ALIAS          NAME
  OXYGEN    C     O2             OXYGEN
  HYDROGEN  C     H2             HYDROGEN
  NITROGEN  C     N2             NITROGEN
  AMMONIA   C     H3N            AMMONIA
  WATER     C     H2O            WATER
  CARBO-01  C     CO2            CARBON-DIOXIDE
  NIACINAM  C     NIACINAMIDE    NIACINAMIDE
  METDIAMI  C     MPDA           MPDA
  METHYLPI  C     METHYLPIPER    METHYLPIPER
  3-MET-01  C     C6H7N-D2       3-METHYLPYRIDINE
  NICOT-01  C     C6H4N2         NICOTINONITRILE
  AMMONICO  C     SALTFORM       SALTFORM
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 10
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  A-101    MODEL: RADFRAC
-------------------------------
   INLETS   - S-112    STAGE  17
   OUTLETS  - S-113    STAGE   1
              S-119    STAGE  20
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           141.441         141.441          0.00000
      MASS(LB/HR   )           3307.12         3307.12        -0.508771E-14
      ENTHALPY(BTU/HR  )     0.158151E+07      458444.          0.710122

                    ***  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  ****
                       **********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                                      20
   ALGORITHM OPTION                                    STANDARD
   ABSORBER OPTION                                     NO
   INITIALIZATION OPTION                               STANDARD
   HYDRAULIC PARAMETER CALCULATIONS                    NO
   INSIDE LOOP CONVERGENCE METHOD                      BROYDEN
   DESIGN SPECIFICATION METHOD                         NESTED
   MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                25
   MAXIMUM NO. OF INSIDE LOOP ITERATIONS                 10
   MAXIMUM NUMBER OF FLASH ITERATIONS                    30
   FLASH TOLERANCE                                        0.000100000
   OUTSIDE LOOP CONVERGENCE TOLERANCE                     0.000100000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 11
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  A-101    MODEL: RADFRAC (CONTINUED)

  ****   COL-SPECS   ****

   MOLAR VAPOR DIST / TOTAL DIST                                  1.00000
   MOLAR REFLUX RATIO                                             1.00000
   DISTILLATE TO FEED RATIO                                       0.79890

  ****    PROFILES   ****

   P-SPEC          STAGE   1  PRES, PSIA                         40.0000

                      *******************
                      ****  RESULTS  ****
                      *******************


  ***   COMPONENT SPLIT FRACTIONS   ***

                           OUTLET STREAMS
                           --------------
               S-113       S-119
   COMPONENT:
   HYDROGEN    1.0000      0.0000
   AMMONIA     1.0000      .37851E-08
   METDIAMI    .10179E-13  1.0000
   METHYLPI    .52024E-05  .99999
   3-MET-01    .53922E-03  .99946


  ***    SUMMARY OF KEY RESULTS    ***

   TOP STAGE TEMPERATURE          F                               5.99019
   BOTTOM STAGE TEMPERATURE       F                             366.260
   TOP STAGE LIQUID FLOW          LBMOL/HR                      112.997
   BOTTOM STAGE LIQUID FLOW       LBMOL/HR                       28.4438
   TOP STAGE VAPOR FLOW           LBMOL/HR                      112.997
   BOILUP VAPOR FLOW              LBMOL/HR                      109.989
   MOLAR REFLUX RATIO                                             1.00000
   MOLAR BOILUP RATIO                                             3.86689
   CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                -2,810,550.
   REBOILER DUTY                  BTU/HR                 1,687,480.

  ****   MAXIMUM FINAL RELATIVE ERRORS   ****

   DEW POINT                       0.29148      STAGE=  2
   BUBBLE POINT                    0.22573      STAGE=  2
   COMPONENT MASS BALANCE          0.23486E-05  STAGE= 13 COMP=HYDROGEN
   ENERGY BALANCE                  0.92543E-04  STAGE=  1
```

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 12
NIACIN PRODUCTION
U-O-S BLOCK SECTION

BLOCK: A-101 MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL LIQUID	ENTHALPY BTU/LBMOL VAPOR	HEAT DUTY BTU/HR
1	5.9902	40.000	9932.9	-5484.0	-.28105+07
2	274.09	40.000	33923.	14662.	
7	323.08	40.000	36404.	29345.	
8	323.12	40.000	36390.	29348.	
9	323.09	40.000	36367.	29340.	
10	323.09	40.000	36340.	29327.	
15	323.15	40.000	36040.	29189.	
16	323.17	40.000	35922.	29135.	
17	365.80	40.000	38156.	53303.	
18	366.20	40.000	38127.	53586.	
19	366.23	40.000	38041.	53527.	
20	366.26	40.000	37904.	53419.	.16875+07

STAGE	FLOW RATE LBMOL/HR LIQUID	FLOW RATE LBMOL/HR VAPOR	FEED RATE LBMOL/HR LIQUID	FEED RATE LBMOL/HR VAPOR	FEED RATE LBMOL/HR MIXED	PRODUCT RATE LBMOL/HR LIQUID	PRODUCT RATE LBMOL/HR VAPOR
1	113.0	113.0					112.9972
2	145.5	226.0					
7	159.5	272.4					
8	159.5	272.5					
9	159.5	272.5					
10	159.5	272.5					
15	159.5	272.5					
16	122.3	272.5		141.4410			
17	138.3	93.84					
18	138.4	109.8					
19	138.4	110.0					
20	28.44	110.0				28.4437	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR LIQUID	FLOW RATE LB/HR VAPOR	FEED RATE LB/HR LIQUID	FEED RATE LB/HR VAPOR	FEED RATE LB/HR MIXED	PRODUCT RATE LB/HR LIQUID	PRODUCT RATE LB/HR VAPOR
1	8255.	656.5					656.4752
2	0.1346E+05	8912.					
7	0.1481E+05	0.1546E+05					
8	0.1481E+05	0.1547E+05					
9	0.1481E+05	0.1547E+05					
10	0.1481E+05	0.1547E+05					

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 13
NIACIN PRODUCTION
U-O-S BLOCK SECTION

BLOCK: A-101 MODEL: RADFRAC (CONTINUED)

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR LIQUID	FLOW RATE LB/HR VAPOR	FEED RATE LB/HR LIQUID	FEED RATE LB/HR VAPOR	FEED RATE LB/HR MIXED	PRODUCT RATE LB/HR LIQUID	PRODUCT RATE LB/HR VAPOR
15	0.1481E+05	0.1547E+05					
16	0.1136E+05	0.1547E+05		3307.1178			
17	0.1288E+05	8708.					
18	0.1290E+05	0.1023E+05					
19	0.1290E+05	0.1025E+05					
20	2651.	0.1025E+05				2650.6425	

**** MOLE-X-PROFILE ****

STAGE	HYDROGEN	AMMONIA	METDIAMI	METHYLPI	3-MET-01
1	0.22988E-03	0.26347	0.81560E-15	0.10944E-03	0.73619
2	0.26305E-03	0.79574E-02	0.49564E-14	0.19282E-03	0.99159
7	0.33770E-03	0.32509E-02	0.33350E-11	0.67972E-03	0.99573
8	0.33737E-03	0.32480E-02	0.12007E-10	0.87216E-03	0.99554
9	0.33778E-03	0.32495E-02	0.43208E-10	0.11190E-02	0.99529
10	0.33783E-03	0.32498E-02	0.15548E-09	0.14356E-02	0.99498
15	0.33809E-03	0.32493E-02	0.93594E-07	0.49794E-02	0.99143
16	0.33818E-03	0.32491E-02	0.33637E-06	0.63814E-02	0.99003
17	0.58234E-06	0.10987E-03	0.32087E-06	0.66858E-02	0.99320
18	0.97070E-09	0.35849E-05	0.36123E-06	0.73383E-02	0.99266
19	0.16180E-11	0.11690E-06	0.51489E-06	0.83714E-02	0.99163
20	0.26969E-14	0.37871E-08	0.10968E-05	0.10005E-01	0.98999

**** MOLE-Y-PROFILE ****

STAGE	HYDROGEN	AMMONIA	METDIAMI	METHYLPI	3-MET-01
1	0.74801	0.25186	0.28103E-20	0.13103E-07	0.13445E-03
2	0.37412	0.25766	0.40780E-15	0.54726E-04	0.36816
7	0.31052	0.10639	0.54206E-12	0.30997E-03	0.58279
8	0.31039	0.10634	0.19520E-11	0.39786E-03	0.58287
9	0.31036	0.10633	0.70281E-11	0.51053E-03	0.58280
10	0.31037	0.10634	0.25291E-10	0.65498E-03	0.58263
15	0.31039	0.10634	0.15238E-07	0.22735E-02	0.58099
16	0.31040	0.10635	0.54781E-07	0.29145E-02	0.58034
17	0.44069E-03	0.42339E-02	0.10587E-06	0.52830E-02	0.99004
18	0.73316E-06	0.13832E-03	0.11991E-06	0.58260E-02	0.99403
19	0.12217E-08	0.45109E-05	0.17100E-06	0.66486E-02	0.99335
20	0.20357E-11	0.14615E-06	0.36440E-06	0.79489E-02	0.99205

**** K-VALUES ****

STAGE	HYDROGEN	AMMONIA	METDIAMI	METHYLPI	3-MET-01
1	3251.8	0.95583	0.34477E-05	0.11976E-03	0.18268E-03
2	1101.1	25.071	0.63709E-01	0.21977	0.28749
7	918.83	32.718	0.16262	0.45615	0.58543
8	918.64	32.725	0.16275	0.45643	0.58579
9	918.70	32.720	0.16266	0.45625	0.58556
10	918.65	32.720	0.16266	0.45625	0.58557
15	917.99	32.726	0.16281	0.45658	0.58601
16	917.72	32.729	0.16286	0.45671	0.58618
17	756.74	38.535	0.32995	0.79019	0.99682

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 14
NIACIN PRODUCTION
U-O-S BLOCK SECTION

BLOCK: A-101 MODEL: RADFRAC (CONTINUED)

**** K-VALUES ****

STAGE	HYDROGEN	AMMONIA	METDIAMI	METHYLPI	3-MET-01
18	755.29	38.586	0.33196	0.79393	1.0014
19	755.09	38.589	0.33210	0.79420	1.0017
20	754.83	38.591	0.33224	0.79447	1.0021

**** MASS-X-PROFILE ****

STAGE	HYDROGEN	AMMONIA	METDIAMI	METHYLPI	3-MET-01
1	0.63430E-05	0.61417E-01	0.12972E-14	0.14855E-03	0.93843
2	0.57328E-05	0.14651E-02	0.62264E-14	0.20672E-03	0.99832
7	0.73315E-05	0.59625E-03	0.41735E-11	0.72596E-03	0.99867
8	0.73242E-05	0.59572E-03	0.15025E-10	0.93147E-03	0.99847
9	0.73330E-05	0.59598E-03	0.54070E-10	0.11951E-02	0.99820
10	0.73340E-05	0.59602E-03	0.19456E-09	0.15331E-02	0.99786
15	0.73379E-05	0.59580E-03	0.11709E-06	0.53166E-02	0.99408
16	0.73393E-05	0.59570E-03	0.42079E-06	0.68129E-02	0.99258
17	0.12601E-07	0.20085E-04	0.40023E-06	0.71170E-02	0.99286
18	0.21002E-10	0.65526E-06	0.45050E-06	0.78106E-02	0.99219
19	0.35005E-13	0.21366E-07	0.64210E-06	0.89097E-02	0.99109
20	0.58341E-16	0.69211E-09	0.13677E-05	0.10647E-01	0.98935

**** MASS-Y-PROFILE ****

STAGE	HYDROGEN	AMMONIA	METDIAMI	METHYLPI	3-MET-01
1	0.25955	0.73829	0.56209E-19	0.22366E-06	0.21552E-02
2	0.19125E-01	0.11128	0.12017E-14	0.13763E-03	0.86946
7	0.11032E-01	0.31931E-01	0.11101E-11	0.54174E-03	0.95650
8	0.11024E-01	0.31909E-01	0.39964E-11	0.69515E-03	0.95637
9	0.11022E-01	0.31903E-01	0.14387E-10	0.89195E-03	0.95618
10	0.11023E-01	0.31906E-01	0.51775E-10	0.11444E-02	0.95593
15	0.11022E-01	0.31903E-01	0.31191E-07	0.39716E-02	0.95310
16	0.11022E-01	0.31902E-01	0.11212E-06	0.50910E-02	0.95199
17	0.95732E-05	0.77703E-03	0.13257E-06	0.56458E-02	0.99357
18	0.15866E-07	0.25289E-04	0.14958E-06	0.62024E-02	0.99377
19	0.26435E-10	0.82457E-06	0.21327E-06	0.70769E-02	0.99292
20	0.44043E-13	0.26713E-07	0.45444E-06	0.84602E-02	0.99154

BLOCK: A-102 MODEL: RADFRAC

INLETS - S-114 STAGE 8
S-117 STAGE 2
OUTLETS - S-115 STAGE 1
S-118 STAGE 10
PROPERTY OPTION SET: RK-SOAVE STANDARD RKS EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 15
NIACIN PRODUCTION
U-O-S BLOCK SECTION

BLOCK: A-102 MODEL: RADFRAC (CONTINUED)

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	179.607	179.607	0.00000
MASS(LB/HR)	1856.48	1856.48	-0.489904E-15
ENTHALPY(BTU/HR)	-0.861937E+07	-0.902541E+07	0.449883E-01

*** 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 ****
****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	10
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	1.00000
MOLAR REFLUX RATIO	1.00000
DISTILLATE TO FEED RATIO	0.47200

**** PROFILES ****

P-SPEC STAGE 1 PRES, PSIA 170.000

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 16
NIACIN PRODUCTION
U-O-S BLOCK SECTION

BLOCK: A-102 MODEL: RADFRAC (CONTINUED)

****
**** RESULTS ****
****

*** COMPONENT SPLIT FRACTIONS ***

COMPONENT:	OUTLET STREAMS S-115	S-118
HYDROGEN	1.0000	0.0000
AMMONIA	.88402E-02	.99116
WATER	.74460E-12	1.0000
METHYLPI	.21064E-01	.97894
3-MET-01	.49702E-05	1.0000

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	F	-117.878
BOTTOM STAGE TEMPERATURE	F	224.723
TOP STAGE LIQUID FLOW	LBMOL/HR	84.7747
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	94.8327
TOP STAGE VAPOR FLOW	LBMOL/HR	84.7747
BOILUP VAPOR FLOW	LBMOL/HR	58.8010
MOLAR REFLUX RATIO		1.00000
MOLAR BOILUP RATIO		0.62005
CONDENSER DUTY (W/O SUBCOOL)	BTU/HR	-1,227,370.
REBOILER DUTY	BTU/HR	821,341.

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.95300E-04	STAGE= 4
BUBBLE POINT	0.35389E-03	STAGE= 4
COMPONENT MASS BALANCE	0.12038E-05	STAGE= 5 COMP=WATER
ENERGY BALANCE	0.57084E-04	STAGE= 10

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 17
NIACIN PRODUCTION
U-O-S BLOCK SECTION

BLOCK: A-102 MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL LIQUID	VAPOR	HEAT DUTY BTU/HR
1	-117.88	170.00	-32439.	-1380.6	-.12274+07
2	90.052	170.00	-67994.	-9671.1	
3	93.909	170.00	-67623.	-10423.	
4	94.146	170.00	-67617.	-10479.	
5	94.117	170.00	-67661.	-10484.	
6	94.485	170.00	-68036.	-10486.	
7	102.22	170.00	-72608.	-10430.	
8	137.92	170.00	-68804.	-19530.	
9	146.90	170.00	-72610.	-19503.	
10	224.72	170.00	-93938.	-24248.	.82134+06

STAGE	FLOW RATE LBMOL/HR LIQUID	VAPOR	FEED RATE LBMOL/HR LIQUID	VAPOR	MIXED	PRODUCT RATE LBMOL/HR LIQUID	VAPOR
1	84.77	84.77					84.7746
2	166.0	169.5	66.6101				
3	167.3	184.2					
4	167.3	185.4					
5	167.2	185.5					
6	165.9	185.3					
7	148.4	184.1		112.9972			
8	159.8	53.58					
9	153.6	65.00					
10	94.83	58.80				94.8326	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR LIQUID	VAPOR	FEED RATE LB/HR LIQUID	VAPOR	MIXED	PRODUCT RATE LB/HR LIQUID	VAPOR
1	1522.	174.7					174.6730
2	2964.	1696.	1200.0000				
3	2980.	1938.					
4	2977.	1954.					
5	2971.	1952.					
6	2942.	1946.					
7	2610.	1917.		656.4752			
8	2816.	928.4					
9	2708.	1134.					
10	1682.	1026.				1681.8022	

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 18
NIACIN PRODUCTION
U-O-S BLOCK SECTION

BLOCK: A-102 MODEL: RADFRAC (CONTINUED)

**** MOLE-X-PROFILE ****

STAGE	HYDROGEN	AMMONIA	WATER	METHYLPI	3-MET-01
1	0.70949E-04	0.98669	0.14060E-02	0.29009E-02	0.89298E-02
2	0.27256E-04	0.59231	0.40213	0.62850E-03	0.49096E-02
3	0.26897E-04	0.59573	0.39912	0.25130E-03	0.48689E-02
4	0.26694E-04	0.59607	0.39904	0.99014E-04	0.47627E-02
5	0.26490E-04	0.59601	0.39935	0.38166E-04	0.45728E-02
6	0.25748E-04	0.59303	0.40291	0.13317E-04	0.40266E-02
7	0.20285E-04	0.54830	0.45018	0.17474E-05	0.14925E-02
8	0.52886E-08	0.57865	0.41905	0.13053E-05	0.22968E-02
9	0.10593E-11	0.53782	0.46034	0.46220E-06	0.18397E-02
10	0.15880E-15	0.29744	0.70240	0.15283E-07	0.16020E-03

**** MOLE-Y-PROFILE ****

STAGE	HYDROGEN	AMMONIA	WATER	METHYLPI	3-MET-01
1	0.99703	0.29677E-02	0.58506E-12	0.36788E-09	0.89070E-09
2	0.49855	0.49483	0.70299E-03	0.14505E-02	0.44649E-02
3	0.45895	0.53525	0.80003E-03	0.56651E-03	0.44254E-02
4	0.45584	0.53873	0.80477E-03	0.22668E-03	0.43919E-02
5	0.45576	0.53905	0.80282E-03	0.89316E-04	0.42962E-02
6	0.45606	0.53896	0.82082E-03	0.34426E-04	0.41247E-02
7	0.45922	0.53587	0.12717E-02	0.12003E-04	0.36293E-02
8	0.56186E-04	0.99230	0.37866E-02	0.48129E-05	0.38505E-02
9	0.13004E-07	0.98890	0.56790E-02	0.31873E-05	0.54138E-02
10	0.27674E-11	0.92550	0.69954E-01	0.11830E-05	0.45482E-02

**** K-VALUES ****

STAGE	HYDROGEN	AMMONIA	WATER	METHYLPI	3-MET-01
1	14051.	0.30077E-02	0.41621E-09	0.12682E-06	0.99751E-07
2	18290.	0.83529	0.17488E-02	2.3091	0.90986
3	17072.	0.89843	0.20044E-02	2.2565	0.90964
4	17090.	0.90379	0.20163E-02	2.2918	0.92296
5	17213.	0.90450	0.20098E-02	2.3409	0.93972
6	17711.	0.90892	0.20368E-02	2.5822	1.0234
7	22629.	0.97729	0.28252E-02	6.8655	2.4305
8	10621.	1.7148	0.90364E-02	3.6851	1.6757
9	12266.	1.8385	0.12337E-01	6.8879	2.9399
10	17431.	3.1117	0.99591E-01	77.422	28.397

**** MASS-X-PROFILE ****

STAGE	HYDROGEN	AMMONIA	WATER	METHYLPI	3-MET-01
1	0.79685E-05	0.93622	0.14112E-02	0.16028E-01	0.46333E-01
2	0.30779E-05	0.56507	0.40582	0.34915E-02	0.25613E-01
3	0.30436E-05	0.56952	0.40362	0.13989E-02	0.25453E-01
4	0.30242E-05	0.57051	0.40401	0.55184E-03	0.24927E-01
5	0.30044E-05	0.57106	0.40476	0.21294E-03	0.23959E-01
6	0.29268E-05	0.56949	0.40929	0.74471E-04	0.21145E-01
7	0.23250E-05	0.53095	0.46114	0.98528E-05	0.79031E-02
8	0.60513E-09	0.55935	0.42850	0.73474E-05	0.12141E-01
9	0.12116E-12	0.51971	0.47056	0.26008E-05	0.97211E-02
10	0.18051E-16	0.28564	0.71352	0.85464E-07	0.84125E-03

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 19
NIACIN PRODUCTION
U-O-S BLOCK SECTION

BLOCK: A-102 MODEL: RADFRAC (CONTINUED)

**** MASS-Y-PROFILE ****

STAGE	HYDROGEN	AMMONIA	WATER	METHYLPI	3-MET-01
1	0.97547	0.24529E-01	0.51154E-11	0.17706E-07	0.40258E-07
2	0.10046	0.84234	0.12659E-02	0.14378E-01	0.41562E-01
3	0.87916E-01	0.86621	0.13696E-02	0.53386E-02	0.39163E-01
4	0.87186E-01	0.87050	0.13756E-02	0.21329E-02	0.38807E-01
5	0.87314E-01	0.87245	0.13745E-02	0.84177E-03	0.38023E-01
6	0.87555E-01	0.87413	0.14083E-02	0.32513E-03	0.36582E-01
7	0.88892E-01	0.87634	0.22000E-02	0.11431E-03	0.32455E-01
8	0.65369E-05	0.97533	0.39370E-02	0.27547E-04	0.20696E-01
9	0.15024E-08	0.96522	0.58635E-02	0.18116E-04	0.28896E-01
10	0.31978E-12	0.90348	0.72238E-01	0.67246E-05	0.24279E-01

BLOCK: B-201 MODEL: COMPR

INLET STREAM: S-208
OUTLET STREAM: S-209
PROPERTY OPTION SET: RK-SOAVE STANDARD RKS EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	4.58096	4.58096	0.00000
MASS(LB/HR)	148.436	148.436	0.191474E-15
ENTHALPY(BTU/HR)	-42755.7	-36941.9	-0.135977

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	7.17771	LB/HR
PRODUCT STREAMS CO2E	7.17771	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 ***

ISENTROPIC CENTRIFUGAL COMPRESSOR

OUTLET PRESSURE PSIA	31.8503
ISENTROPIC EFFICIENCY	0.72000
MECHANICAL EFFICIENCY	1.00000

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                         03/27/2013  PAGE 20
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  B-201    MODEL: COMPR (CONTINUED)

                          ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                   2.28491
   BRAKE      HORSEPOWER REQUIREMENT  HP                   2.28491
   NET WORK REQUIRED                  HP                   2.28491
   POWER LOSSES                       HP                   0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                   1.64514
   CALCULATED OUTLET TEMP  F                             249.416
   ISENTROPIC TEMPERATURE  F                             201.909
   EFFICIENCY (POLYTR/ISENTR) USED                         0.72000
   OUTLET VAPOR FRACTION                                   1.00000
   HEAD DEVELOPED,       FT-LBF/LB                    21,944.6
   MECHANICAL EFFICIENCY USED                              1.00000
   INLET HEAT CAPACITY RATIO                               1.38030
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                1,789.30
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                1,094.11
   INLET  COMPRESSIBILITY FACTOR                           0.99898
   OUTLET COMPRESSIBILITY FACTOR                           0.99968
   AV. ISENT. VOL. EXPONENT                                1.37328
   AV. ISENT. TEMP EXPONENT                                1.37237
   AV. ACTUAL VOL. EXPONENT                                1.56780
   AV. ACTUAL TEMP EXPONENT                                1.56558

BLOCK:  B-202    MODEL: COMPR
-----------------------------
  INLET STREAM:          S-215
  OUTLET STREAM:         S-216
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          4.57472         4.57472         0.00000
      MASS(LB/HR   )          148.240         148.240         0.00000
      ENTHALPY(BTU/HR  )     -42211.3        -37111.0        -0.120827
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                         03/27/2013  PAGE 21
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  B-202    MODEL: COMPR (CONTINUED)

                      ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E              7.16881      LB/HR
   PRODUCT STREAMS CO2E           7.16881      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  ***

  ISENTROPIC CENTRIFUGAL COMPRESSOR
   PRESSURE CHANGE  PSI                                   15.0000
   ISENTROPIC EFFICIENCY                                   0.72000
   MECHANICAL EFFICIENCY                                   1.00000

                          ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                   2.00448
   BRAKE      HORSEPOWER REQUIREMENT  HP                   2.00448
   NET WORK REQUIRED                  HP                   2.00448
   POWER LOSSES                       HP                   0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                   1.44323
   CALCULATED OUTLET PRES  PSIA                           30.2298
   CALCULATED OUTLET TEMP  F                             228.908
   ISENTROPIC TEMPERATURE  F                             186.982
   EFFICIENCY (POLYTR/ISENTR) USED                         0.72000
   OUTLET VAPOR FRACTION                                   1.00000
   HEAD DEVELOPED,       FT-LBF/LB                    19,276.8
   MECHANICAL EFFICIENCY USED                              1.00000
   INLET HEAT CAPACITY RATIO                               1.38076
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                1,728.16
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                1,117.79
   INLET  COMPRESSIBILITY FACTOR                           0.99896
   OUTLET COMPRESSIBILITY FACTOR                           0.99959
   AV. ISENT. VOL. EXPONENT                                1.37437
   AV. ISENT. TEMP EXPONENT                                1.37348
   AV. ACTUAL VOL. EXPONENT                                1.57349
   AV. ACTUAL TEMP EXPONENT                                1.57123
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 22
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  B-203    MODEL: COMPR
-----------------------------
  INLET STREAM:         S-222
  OUTLET STREAM:        S-223
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          4.56887         4.56887         0.00000
      MASS(LB/HR   )          148.056         148.056         0.00000
      ENTHALPY(BTU/HR  )     -41700.4        -35024.6        -0.160091

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           7.15993      LB/HR
   PRODUCT STREAMS CO2E        7.15993      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  ***

  ISENTROPIC CENTRIFUGAL COMPRESSOR
   PRESSURE CHANGE  PSI                                      22.0000
   ISENTROPIC EFFICIENCY                                      0.72000
   MECHANICAL EFFICIENCY                                      1.00000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 23
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  B-203    MODEL: COMPR (CONTINUED)

                          ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                        2.62371
   BRAKE      HORSEPOWER REQUIREMENT  HP                        2.62371
   NET WORK REQUIRED                  HP                        2.62371
   POWER LOSSES                       HP                        0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                        1.88907
   CALCULATED OUTLET PRES  PSIA                                37.7298
   CALCULATED OUTLET TEMP  F                                  275.301
   ISENTROPIC TEMPERATURE  F                                  220.783
   EFFICIENCY (POLYTR/ISENTR) USED                              0.72000
   OUTLET VAPOR FRACTION                                        1.00000
   HEAD DEVELOPED,        FT-LBF/LB                        25,263.2
   MECHANICAL EFFICIENCY USED                                   1.00000
   INLET HEAT CAPACITY RATIO                                    1.38119
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                     1,671.05
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                       954.928
   INLET  COMPRESSIBILITY FACTOR                                0.99894
   OUTLET COMPRESSIBILITY FACTOR                                0.99982
   AV. ISENT. VOL. EXPONENT                                     1.37341
   AV. ISENT. TEMP EXPONENT                                     1.37234
   AV. ACTUAL VOL. EXPONENT                                     1.56352
   AV. ACTUAL TEMP EXPONENT                                     1.56107

BLOCK:  C-101    MODEL: COMPR
-----------------------------
  INLET STREAM:         S-104
  OUTLET STREAM:        S-105
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          28.7464         28.7464         0.00000
      MASS(LB/HR   )          3340.34         3340.34         0.00000
      ENTHALPY(BTU/HR  )     -579387.        -522590.        -0.980286E-01

                   ***  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
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                         03/27/2013  PAGE 24
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  C-101    MODEL: COMPR (CONTINUED)

                         ***  INPUT DATA  ***

  ISENTROPIC CENTRIFUGAL COMPRESSOR
   OUTLET PRESSURE  PSIA                                         72.5189
   ISENTROPIC EFFICIENCY                                          0.72000
   MECHANICAL EFFICIENCY                                          1.00000

                         ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                         22.3219
   BRAKE      HORSEPOWER REQUIREMENT  HP                         22.3219
   NET WORK REQUIRED                  HP                         22.3219
   POWER LOSSES                       HP                          0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                         16.0717
   CALCULATED OUTLET TEMP  F                                    560.209
   ISENTROPIC TEMPERATURE  F                                    552.594
   EFFICIENCY (POLYTR/ISENTR) USED                                0.72000
   OUTLET VAPOR FRACTION                                          1.00000
   HEAD DEVELOPED,        FT-LBF/LB                           9,526.59
   MECHANICAL EFFICIENCY USED                                     1.00000
   INLET HEAT CAPACITY RATIO                                      1.03692
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                       8,642.49
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                       3,915.22
   INLET  COMPRESSIBILITY FACTOR                                  0.95152
   OUTLET COMPRESSIBILITY FACTOR                                  0.90244
   AV. ISENT. VOL. EXPONENT                                       0.96197
   AV. ISENT. TEMP EXPONENT                                       1.03431
   AV. ACTUAL VOL. EXPONENT                                       0.97492
   AV. ACTUAL TEMP EXPONENT                                       1.04480

BLOCK:  C-102    MODEL: COMPR
-----------------------------
  INLET STREAM:           S-107
  OUTLET STREAM:          S-110
  PROPERTY OPTION SET:    RK-SOAVE  STANDARD RKS EQUATION OF STATE
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                         03/27/2013  PAGE 25
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  C-102    MODEL: COMPR (CONTINUED)

                         ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT          RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)             56.9179          56.9179          0.00000
      MASS(LB/HR   )             3306.95          3306.95          0.00000
      ENTHALPY(BTU/HR  )      -0.150170E+07    -0.131410E+07    -0.124925

                         ***  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  ***

  ISENTROPIC CENTRIFUGAL COMPRESSOR
   OUTLET PRESSURE  PSIA                                         72.5189
   ISENTROPIC EFFICIENCY                                          0.72000
   MECHANICAL EFFICIENCY                                          1.00000

                         ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                         73.7292
   BRAKE      HORSEPOWER REQUIREMENT  HP                         73.7292
   NET WORK REQUIRED                  HP                         73.7292
   POWER LOSSES                       HP                          0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                         53.0850
   CALCULATED OUTLET TEMP  F                                    393.178
   ISENTROPIC TEMPERATURE  F                                    374.057
   EFFICIENCY (POLYTR/ISENTR) USED                                0.72000
   OUTLET VAPOR FRACTION                                          1.00000
   HEAD DEVELOPED,        FT-LBF/LB                          31,784.1
   MECHANICAL EFFICIENCY USED                                     1.00000
   INLET HEAT CAPACITY RATIO                                      1.08913
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                      29,719.9
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                       6,847.95
   INLET  COMPRESSIBILITY FACTOR                                  0.98498
   OUTLET COMPRESSIBILITY FACTOR                                  0.95331
   AV. ISENT. VOL. EXPONENT                                       1.05274
   AV. ISENT. TEMP EXPONENT                                       1.09495
   AV. ACTUAL VOL. EXPONENT                                       1.08748
   AV. ACTUAL TEMP EXPONENT                                       1.11225
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 26
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  C-102    MODEL: COMPR (CONTINUED)

BLOCK:  C-103    MODEL: COMPR
-----------------------------
  INLET STREAM:          S-113
  OUTLET STREAM:         S-114
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                IN             OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          112.997        112.997        0.00000
      MASS(LB/HR   )          656.475        656.475       -0.173178E-15
      ENTHALPY(BTU/HR  )     -619677.       -361903.       -0.415982

                  ***  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  ***

  ISENTROPIC CENTRIFUGAL COMPRESSOR
   OUTLET PRESSURE  PSIA                                 170.000
   ISENTROPIC EFFICIENCY                                   0.72000
   MECHANICAL EFFICIENCY                                   1.00000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 27
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  C-103    MODEL: COMPR (CONTINUED)

                           ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                  101.309
   BRAKE      HORSEPOWER REQUIREMENT  HP                  101.309
   NET WORK REQUIRED                  HP                  101.309
   POWER LOSSES                       HP                    0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                   72.9426
   CALCULATED OUTLET TEMP  F                              313.672
   ISENTROPIC TEMPERATURE  F                              229.872
   EFFICIENCY (POLYTR/ISENTR) USED                          0.72000
   OUTLET VAPOR FRACTION                                    1.00000
   HEAD DEVELOPED,        FT-LBF/LB                   220,003.
   MECHANICAL EFFICIENCY USED                               1.00000
   INLET HEAT CAPACITY RATIO                                1.38803
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                14,104.1
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                 5,536.64
   INLET  COMPRESSIBILITY FACTOR                            0.99911
   OUTLET COMPRESSIBILITY FACTOR                            1.00369
   AV. ISENT. VOL. EXPONENT                                 1.37758
   AV. ISENT. TEMP EXPONENT                                 1.37234
   AV. ACTUAL VOL. EXPONENT                                 1.54738
   AV. ACTUAL TEMP EXPONENT                                 1.53984

BLOCK:  C-301    MODEL: COMPR
-----------------------------
  INLET STREAM:          S-310
  OUTLET STREAM:         S-311
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                IN             OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          1241.79        1241.79        0.00000
      MASS(LB/HR   )          22481.2        22481.2        0.00000
      ENTHALPY(BTU/HR  )   -0.124572E+09  -0.119198E+09  -0.431451E-01

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           3.46806      LB/HR
   PRODUCT STREAMS CO2E        3.46806      LB/HR
   NET STREAMS CO2E PRODUCTION 0.00000      LB/HR
   UTILITIES CO2E PRODUCTION   0.00000      LB/HR
   TOTAL CO2E PRODUCTION       0.00000      LB/HR
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                     03/27/2013  PAGE 28
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  C-301    MODEL: COMPR (CONTINUED)

                         ***  INPUT DATA  ***

  ISENTROPIC CENTRIFUGAL COMPRESSOR
   OUTLET PRESSURE  PSIA                                       68.0082
   ISENTROPIC EFFICIENCY                                        0.72000
   MECHANICAL EFFICIENCY                                        1.00000

                         ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                   2,112.33
   BRAKE      HORSEPOWER REQUIREMENT  HP                   2,112.33
   NET WORK REQUIRED                  HP                   2,112.33
   POWER LOSSES                       HP                       0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                   1,520.88
   CALCULATED OUTLET TEMP  F                                 887.201
   ISENTROPIC TEMPERATURE  F                                 753.361
   EFFICIENCY (POLYTR/ISENTR) USED                              0.72000
   OUTLET VAPOR FRACTION                                        1.00000
   HEAD DEVELOPED,       FT-LBF/LB                        133,949.
   MECHANICAL EFFICIENCY USED                                   1.00000
   INLET HEAT CAPACITY RATIO                                    1.31829
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                   774,892.
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                   262,833.
   INLET  COMPRESSIBILITY FACTOR                                0.99577
   OUTLET COMPRESSIBILITY FACTOR                                0.99589
   AV. ISENT. VOL. EXPONENT                                     1.30096
   AV. ISENT. TEMP EXPONENT                                     1.30308
   AV. ACTUAL VOL. EXPONENT                                     1.42936
   AV. ACTUAL TEMP EXPONENT                                     1.42920

BLOCK:  D-101    MODEL: RADFRAC
-------------------------------
   INLETS   - S-106    STAGE  33
   OUTLETS  - S-107    STAGE   1
              S-108    STAGE  40
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                     03/27/2013  PAGE 29
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  D-101    MODEL: RADFRAC (CONTINUED)

                         ***  MASS AND ENERGY BALANCE  ***
                                     IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)              57.2054          57.2054      -0.582540E-13
      MASS(LB/HR   )              3340.35          3340.35       0.102294E-11
      ENTHALPY(BTU/HR  )         -974645.     -0.151549E+07      0.356876

                         ***  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  ****
                          **********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                                           40
   ALGORITHM OPTION                                         STANDARD
   ABSORBER OPTION                                          NO
   INITIALIZATION OPTION                                    STANDARD
   HYDRAULIC PARAMETER CALCULATIONS                         NO
   INSIDE LOOP CONVERGENCE METHOD                           BROYDEN
   DESIGN SPECIFICATION METHOD                              NESTED
   MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                     25
   MAXIMUM NO. OF INSIDE LOOP ITERATIONS                      10
   MAXIMUM NUMBER OF FLASH ITERATIONS                         30
   FLASH TOLERANCE                                             0.000100000
   OUTSIDE LOOP CONVERGENCE TOLERANCE                          0.000100000

  ****   COL-SPECS   ****

   MOLAR VAPOR DIST / TOTAL DIST                               1.00000
   MOLAR REFLUX RATIO                                          6.41830
   DISTILLATE TO FEED RATIO                                    0.99497
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                       03/27/2013  PAGE 30
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  D-101    MODEL: RADFRAC (CONTINUED)

  ****    PROFILES   ****

   P-SPEC         STAGE   1  PRES, PSIA                      14.6959

                         *******************
                         ****  RESULTS  ****
                         *******************

  ***   COMPONENT SPLIT FRACTIONS   ***

                              OUTLET STREAMS
                              --------------
                 S-107         S-108
   COMPONENT:
   AMMONIA     1.0000        0.0000
   METDIAMI    .10853E-03    .99989
   METHYLPI    1.0000        .11106E-05

  ***    SUMMARY OF KEY RESULTS    ***

   TOP STAGE TEMPERATURE         F                          266.285
   BOTTOM STAGE TEMPERATURE      F                          402.319
   TOP STAGE LIQUID FLOW         LBMOL/HR                   365.316
   BOTTOM STAGE LIQUID FLOW      LBMOL/HR                     0.28746
   TOP STAGE VAPOR FLOW          LBMOL/HR                    56.9179
   BOILUP VAPOR FLOW             LBMOL/HR                   326.461
   MOLAR REFLUX RATIO                                         6.41830
   MOLAR BOILUP RATIO                                     1,135.66
   CONDENSER DUTY (W/O SUBCOOL)  BTU/HR              -6,944,570.
   REBOILER DUTY                 BTU/HR               6,403,730.

  ****   MAXIMUM FINAL RELATIVE ERRORS    ****

   DEW POINT                      0.15416E-05  STAGE= 14
   BUBBLE POINT                   0.39092E-05  STAGE= 14
   COMPONENT MASS BALANCE         0.34000E-05  STAGE= 14 COMP=AMMONIA
   ENERGY BALANCE                 0.10537E-05  STAGE= 14
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                       03/27/2013  PAGE 31
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  D-101    MODEL: RADFRAC (CONTINUED)

  ****    PROFILES   ****

  **NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS
           FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

                                              ENTHALPY
STAGE TEMPERATURE    PRESSURE                BTU/LBMOL          HEAT DUTY
      F              PSIA            LIQUID        VAPOR         BTU/HR

  1   266.28         14.696         -51733.       -26384.       -.69446+07
  2   306.22         14.846         -49716.       -31869.
  5   309.19         15.296         -49553.       -31944.
  6   309.88         15.446         -49517.       -31916.
  7   310.60         15.596         -49484.       -31888.
  8   311.43         15.746         -49458.       -31855.
 31   386.39         19.196         -48982.       -28471.
 32   386.92         19.346         -48938.       -28442.
 33   395.91         19.496         -48373.       -28778.
 39   401.78         20.396         -48005.       -28421.
 40   402.32         20.546         -47961.       -28389.        .64037+07

STAGE     FLOW RATE                FEED RATE                PRODUCT RATE
          LBMOL/HR                 LBMOL/HR                  LBMOL/HR
    LIQUID     VAPOR       LIQUID    VAPOR     MIXED       LIQUID    VAPOR
  1  365.3     56.92                                                56.9179
  2  409.9     422.2
  5  411.6     468.4
  6  411.7     468.5
  7  411.6     468.6
  8  411.0     468.5
 31  343.8     400.6
 32  317.9     400.7               57.2054
 33  325.1     317.6
 39  326.7     326.3
 40 0.2875     326.5                                      0.2874

   ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE                FEED RATE                PRODUCT RATE
          LB/HR                    LB/HR                     LB/HR
    LIQUID     VAPOR       LIQUID    VAPOR     MIXED       LIQUID    VAPOR
  1 0.3599E+05  3307.                                              3306.9499
  2 0.4062E+05 0.3930E+05
  5 0.4079E+05 0.4408E+05
  6 0.4080E+05 0.4410E+05
  7 0.4080E+05 0.4411E+05
  8 0.4077E+05 0.4411E+05
 31 0.3956E+05 0.4284E+05
 32 0.3658E+05 0.4286E+05           3340.3527
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 32
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  D-101    MODEL: RADFRAC (CONTINUED)

   ****  MASS FLOW PROFILES  ****

STAGE     FLOW RATE                  FEED RATE                  PRODUCT RATE
            LB/HR                      LB/HR                        LB/HR
      LIQUID     VAPOR       LIQUID    VAPOR    MIXED        LIQUID    VAPOR
 33 0.3762E+05 0.3654E+05
 39 0.3797E+05 0.3791E+05
 40  33.40      0.3793E+05                                    33.4028

                          ****   MOLE-X-PROFILE     ****
  STAGE     AMMONIA       METDIAMI      METHYLPI
     1     0.79071E-02   0.39850E-05   0.99209
     2     0.95160E-03   0.11640E-04   0.99904
     5     0.79965E-03   0.26825E-03   0.99893
     6     0.80451E-03   0.75651E-03   0.99844
     7     0.80931E-03   0.21249E-02   0.99707
     8     0.81397E-03   0.59324E-02   0.99325
    31     0.86610E-03   0.93667       0.62466E-01
    32     0.87107E-03   0.93651       0.62622E-01
    33     0.10405E-04   0.97118       0.28806E-01
    39     0.33006E-16   0.99976       0.24326E-03
    40     0.40808E-18   0.99989       0.10995E-03

                          ****   MOLE-Y-PROFILE     ****
  STAGE     AMMONIA       METDIAMI      METHYLPI
     1     0.50000       0.54812E-06   0.50000
     2     0.74242E-01   0.35217E-05   0.92575
     5     0.61460E-01   0.83316E-04   0.93846
     6     0.61444E-01   0.23573E-03   0.93832
     7     0.61438E-01   0.66469E-03   0.93790
     8     0.61455E-01   0.18668E-02   0.93668
    31     0.71788E-01   0.80371       0.12451
    32     0.71761E-01   0.80363       0.12461
    33     0.87186E-03   0.93645       0.62678E-01
    39     0.26875E-14   0.99946       0.53926E-03
    40     0.33034E-16   0.99976       0.24338E-03

                          ****   K-VALUES           ****
  STAGE     AMMONIA       METDIAMI      METHYLPI
     1      63.235       0.13754       0.50399
     2      78.018       0.30256       0.92665
     5      76.858       0.31059       0.93946
     6      76.375       0.31159       0.93979
     7      75.914       0.31282       0.94066
     8      75.500       0.31467       0.94304
    31      82.887       0.85805        1.9932
    32      82.383       0.85811        1.9899
    33      83.795       0.96424        2.1758
    39      81.424       0.99970        2.2168
    40      80.951       0.99987        2.2136
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 33
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  D-101    MODEL: RADFRAC (CONTINUED)

                          ****   MASS-X-PROFILE     ****
  STAGE     AMMONIA       METDIAMI      METHYLPI
     1     0.13668E-02   0.47002E-05   0.99863
     2     0.16355E-03   0.13649E-04   0.99982
     5     0.13741E-03   0.31451E-03   0.99955
     6     0.13823E-03   0.88690E-03   0.99897
     7     0.13903E-03   0.24905E-02   0.99737
     8     0.13974E-03   0.69488E-02   0.99291
    31     0.12821E-03   0.94603       0.53844E-01
    32     0.12895E-03   0.94589       0.53980E-01
    33     0.15314E-05   0.97531       0.24689E-01
    39     0.48376E-17   0.99979       0.20762E-03
    40     0.59810E-19   0.99991       0.93837E-04

                          ****   MASS-Y-PROFILE     ****
  STAGE     AMMONIA       METDIAMI      METHYLPI
     1     0.14656       0.10962E-05   0.85344
     2     0.13585E-01   0.43969E-05   0.98641
     5     0.11120E-01   0.10286E-03   0.98878
     6     0.11117E-01   0.29100E-03   0.98859
     7     0.11115E-01   0.82050E-03   0.98806
     8     0.11116E-01   0.23039E-02   0.98658
    31     0.11430E-01   0.87313       0.11544
    32     0.11426E-01   0.87304       0.11553
    33     0.12906E-03   0.94584       0.54029E-01
    39     0.39391E-15   0.99954       0.46026E-03
    40     0.48418E-17   0.99979       0.20772E-03

BLOCK:  DC-301   MODEL: SSPLIT
------------------------------
  INLET STREAM:          S-302
  OUTLET STREAMS:        S-304      S-303
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN                OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1259.04           1259.04         0.00000
      MASS(LB/HR   )            25618.8           25618.8         0.00000
      ENTHALPY(BTU/HR  )      -0.153808E+09   -0.153808E+09   -0.598727E-13

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.365887      LB/HR
   PRODUCT STREAMS CO2E        0.365887      LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 34
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  DC-301   MODEL: SSPLIT (CONTINUED)

                         ***  INPUT DATA  ***

 PRESSURE DROP   PSIA                                     -5.00000

 FRACTION OF FLOW
  SUBSTRM=          STRM=           FRAC=
           MIXED          S-304                  1.00000
           CIPSD          S-304                  0.0

                          ***  RESULTS  ***

 STRM= S-304      SUBSTRM= MIXED    SPLIT FRACT=          1.00000
                           CIPSD                          0.0

 STRM= S-303      SUBSTRM= MIXED    SPLIT FRACT=          0.0
                           CIPSD                          1.00000

BLOCK:  DR-301   MODEL: SEP
---------------------------
  INLET STREAMS:         S-309       S-315       S-307
  OUTLET STREAMS:        S-310       S-316
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1270.20         1270.20       0.179006E-15
      MASS(LB/HR   )           25932.8         25932.8      -0.140285E-15
      ENTHALPY(BTU/HR  )     -0.124897E+09   -0.125748E+09   0.676808E-02

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E          3.46806      LB/HR
   PRODUCT STREAMS CO2E       3.46806      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  ***

  INLET PRESSURE DROP   PSI                                 5.00000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 35
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  DR-301   MODEL: SEP (CONTINUED)

  FLASH SPECS FOR STREAM S-310
  TWO    PHASE  TP  FLASH
  PRESSURE DROP          PSI                               0.0
  MAXIMUM NO. ITERATIONS                                  30
  CONVERGENCE TOLERANCE                                    0.000100000

  FLASH SPECS FOR STREAM S-316
  TWO    PHASE  TP  FLASH
  PRESSURE DROP          PSI                               0.0
  MAXIMUM NO. ITERATIONS                                  30
  CONVERGENCE TOLERANCE                                    0.000100000

  FRACTION OF FEED
    SUBSTREAM= MIXED
      STREAM= S-310     CPT= OXYGEN    FRACTION=          1.00000
                             HYDROGEN                     1.00000
                             NITROGEN                     1.00000
                             AMMONIA                      1.00000
                             WATER                        1.00000
                             CARBO-01                     1.00000
                             NIACINAM                     0.0
                             METDIAMI                     0.0
                             METHYLPI                     0.0
                             3-MET-01                     0.0
                             NICOT-01                     0.0
                             AMMONICO                     0.0

                          ***  RESULTS  ***

  HEAT DUTY              BTU/HR                           -0.85108E+06

 COMPONENT = OXYGEN
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-310      MIXED               1.00000

 COMPONENT = NITROGEN
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-310      MIXED               1.00000

 COMPONENT = AMMONIA
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-310      MIXED               1.00000

 COMPONENT = WATER
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-310      MIXED               1.00000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                   03/27/2013  PAGE 36
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  DR-301   MODEL: SEP (CONTINUED)

 COMPONENT = CARBO-01
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-310      MIXED                 1.00000

 COMPONENT = NIACINAM
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-316      MIXED                 1.00000

 COMPONENT = METDIAMI
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-316      MIXED                 1.00000

 COMPONENT = METHYLPI
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-316      MIXED                 1.00000

 COMPONENT = 3-MET-01
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-316      MIXED                 1.00000

 COMPONENT = NICOT-01
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-316      MIXED                 1.00000

BLOCK:  F-201    MODEL: FLASH2
-------------------------------
  INLET STREAM:          S-227
  OUTLET VAPOR STREAM:   S-228
  OUTLET LIQUID STREAM:  S-229
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                IN            OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          154.898       154.898       0.00000
      MASS(LB/HR   )          5795.22       5795.22      -0.191612E-09
      ENTHALPY(BTU/HR  )   -0.167907E+08  -0.167906E+08  -0.614923E-05

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E              7.43964      LB/HR
   PRODUCT STREAMS CO2E           7.43964      LB/HR
   NET STREAMS CO2E PRODUCTION -0.353994E-06  LB/HR
   UTILITIES CO2E PRODUCTION      0.00000      LB/HR
   TOTAL CO2E PRODUCTION       -0.353994E-06  LB/HR
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                   03/27/2013  PAGE 37
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  F-201    MODEL: FLASH2 (CONTINUED)

                         ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE F                                  32.0000
  SPECIFIED PRESSURE    PSIA                               15.0000
  MAXIMUM NO. ITERATIONS                                   30
  CONVERGENCE TOLERANCE                                     0.000100000

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                   32.000
  OUTLET PRESSURE       PSIA                                15.000
  HEAT DUTY             BTU/HR                              103.25
  VAPOR FRACTION                                            0.28725E-01


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)          K(I)
     OXYGEN        0.27373E-01   0.44082E-04   0.95146        21584.
     NITROGEN      0.90944E-04   0.12611E-07   0.31656E-02
0.25102E+06
     AMMONIA       0.29921E-04   0.30292E-04   0.17386E-04   0.57393
     WATER         0.78787       0.81100       0.57580E-02   0.70998E-
02
     CARBO-01      0.10913E-02   0.52378E-04   0.36222E-01    691.56
     NIACINAM      0.17827       0.18354       0.21623E-07   0.11782E-
06
     METDIAMI      0.20141E-06   0.20363E-06   0.12618E-06   0.61969
     METHYLPI      0.18373E-02   0.18171E-02   0.25191E-02    1.3865
     3-MET-01      0.16370E-02   0.16620E-02   0.79031E-03   0.47554
     NICOT-01      0.18007E-02   0.18518E-02   0.71357E-04   0.38536E-
01

BLOCK:  F-301    MODEL: FLASH2
-------------------------------
  INLET STREAM:          S-312
  OUTLET VAPOR STREAM:   S-313
  OUTLET LIQUID STREAM:  S-317
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                IN            OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          1241.79       1241.79       0.328156E-11
      MASS(LB/HR   )          22481.2       22481.2       0.532414E-11
      ENTHALPY(BTU/HR  )   -0.153812E+09  -0.153812E+09  -0.628592E-09
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 38
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  F-301    MODEL: FLASH2 (CONTINUED)

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            3.46806      LB/HR
   PRODUCT STREAMS CO2E         3.46806      LB/HR
   NET STREAMS CO2E PRODUCTION -0.141470E-08  LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION       -0.141470E-08  LB/HR

                      ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE F                                    32.0000
  PRESSURE DROP         PSI                                   0.0
  MAXIMUM NO. ITERATIONS                                     30
  CONVERGENCE TOLERANCE                                       0.000100000

                       ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                      32.000
  OUTLET PRESSURE       PSIA                                   58.008
  HEAT DUTY             BTU/HR                                 0.96815E-01
  VAPOR FRACTION                                               0.90036E-02


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)          K(I)
     OXYGEN          0.53407E-04   0.19036E-07   0.59297E-02
0.31150E+06
     NITROGEN        0.88768E-02   0.65762E-07   0.98592
0.14992E+08
     AMMONIA         0.25354E-02   0.25571E-02   0.14363E-03   0.56168E-
01
     WATER           0.98847       0.99744       0.10054E-02   0.10080E-
02
     CARBO-01        0.63459E-04   0.39145E-06   0.70051E-02    17895.

BLOCK:  HX-101   MODEL: HEATER
------------------------------
  INLET STREAM:          S-103
  OUTLET STREAM:         S-104
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                 IN            OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          28.7464        28.7464        0.00000
      MASS(LB/HR   )          3340.34        3340.34        0.00000
      ENTHALPY(BTU/HR  )    -0.204694E+07   -579387.       -0.716950
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 39
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  HX-101   MODEL: HEATER (CONTINUED)

                  ***  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                        527.000
  PRESSURE DROP                       PSI                       10.0000
  MAXIMUM NO. ITERATIONS                                        30
  CONVERGENCE TOLERANCE                                          0.000100000


                       ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                     527.00
  OUTLET PRESSURE       PSIA                                   33.511
  HEAT DUTY             BTU/HR                                 0.14676E+07
  OUTLET VAPOR FRACTION                                        1.0000
  PRESSURE-DROP CORRELATION PARAMETER                          0.47894E+07


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)          K(I)
     METDIAMI        1.0000        1.0000        1.0000        2.4346
     METHYLPI        0.10995E-05   0.66282E-06   0.10995E-05   4.0386

BLOCK:  HX-102   MODEL: HEATER
------------------------------
  INLET STREAM:          S-110
  OUTLET STREAM:         S-111
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                 IN            OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          56.9179        56.9179        0.00000
      MASS(LB/HR   )          3306.95        3306.95        0.00000
      ENTHALPY(BTU/HR  )    -0.131410E+07   -0.102115E+07   -0.222926
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                      03/27/2013  PAGE 40
                             NIACIN PRODUCTION
                              U-O-S BLOCK SECTION

BLOCK:  HX-102   MODEL: HEATER (CONTINUED)

                     ***  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                        554.000
  PRESSURE DROP                      PSI                       10.0000
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000


                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                   554.00
  OUTLET PRESSURE       PSIA                                62.519
  HEAT DUTY             BTU/HR                              0.29295E+06
  OUTLET VAPOR FRACTION                                      1.0000
  PRESSURE-DROP CORRELATION PARAMETER                       0.25453E+07


  V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     AMMONIA         0.50000       0.71600E-01   0.50000       34.521
     METDIAMI        0.54812E-06   0.16117E-05   0.54812E-06   1.6812
     METHYLPI        0.50000       0.92840       0.50000       2.6624

BLOCK:  HX-201   MODEL: HEATER
------------------------------
  INLET STREAM:          S-203A
  OUTLET STREAM:         S-203
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)             122.233         122.233         0.00000
      MASS(LB/HR   )             4313.94         4313.94         0.00000
      ENTHALPY(BTU/HR  )      -0.773225E+07   -0.513195E+07   -0.336294
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                      03/27/2013  PAGE 41
                             NIACIN PRODUCTION
                              U-O-S BLOCK SECTION

BLOCK:  HX-201   MODEL: HEATER (CONTINUED)

                     ***  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                        626.000
  PRESSURE DROP                      PSI                       10.0000
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000


                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                   626.00
  OUTLET PRESSURE       PSIA                                30.000
  HEAT DUTY             BTU/HR                              0.26003E+07
  OUTLET VAPOR FRACTION                                      1.0000
  PRESSURE-DROP CORRELATION PARAMETER                       0.66517E+06


  V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     AMMONIA         0.22823       0.13094       0.22823       53.861
     WATER           0.53895       0.43342       0.53895       38.426
     METDIAMI        0.25523E-06   0.67768E-06   0.25523E-06   11.639
     METHYLPI        0.23282E-02   0.48532E-02   0.23282E-02   14.825
     3-MET-01        0.23050       0.43078       0.23050       16.535

BLOCK:  HX-202A  MODEL: HEATER
------------------------------
  INLET STREAM:          S-205
  OUTLET STREAM:         S-206A
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

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

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                    03/27/2013  PAGE 42
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  HX-202A  MODEL: HEATER (CONTINUED)
   TOTAL BALANCE
      MOLE(LBMOL/HR)           182.512         182.512          0.00000
      MASS(LB/HR   )           5795.40         5795.40          0.00000
      ENTHALPY(BTU/HR  )     -0.110133E+08   -0.153902E+08     0.284391

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E              7.43964      LB/HR
   PRODUCT STREAMS CO2E           7.43964      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                      100.000
  PRESSURE DROP                         PSI                      5.00000
  MAXIMUM NO. ITERATIONS                                        30
  CONVERGENCE TOLERANCE                                          0.000100000


                       ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                    100.00
  OUTLET PRESSURE       PSIA                                 24.130
  HEAT DUTY             BTU/HR                              -0.43768E+07
  OUTLET VAPOR FRACTION                                      0.25426E-01
  PRESSURE-DROP CORRELATION PARAMETER                        0.16262E+06


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)          K(I)
     OXYGEN           0.23232E-01   0.20280E-03   0.90593       4467.3
     NITROGEN         0.77185E-04   0.11713E-06   0.30312E-02   25880.
     AMMONIA          0.25394E-04   0.25200E-04   0.32833E-04   1.3029
     WATER            0.81997       0.83992       0.55258E-01   0.65788E-
01
     CARBO-01         0.92621E-03   0.10069E-03   0.32569E-01    323.47
     METDIAMI         0.17093E-06   0.17497E-06   0.16314E-07   0.93248E-
01
     METHYLPI         0.15593E-02   0.15884E-02   0.44202E-03   0.27829
     3-MET-01         0.13893E-02   0.14191E-02   0.24813E-03   0.17486
     NICOT-01         0.15283       0.15675       0.24922E-02   0.15901E-
01

BLOCK:  HX-202B  MODEL: HEATER
------------------------------
  INLET STREAM:          S-206A
  OUTLET STREAM:         S-206
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                    03/27/2013  PAGE 43
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  HX-202B  MODEL: HEATER (CONTINUED)

                  ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           182.512         182.512          0.00000
      MASS(LB/HR   )           5795.40         5795.40          0.00000
      ENTHALPY(BTU/HR  )     -0.153902E+08   -0.154853E+08     0.614673E-02

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E              7.43964      LB/HR
   PRODUCT STREAMS CO2E           7.43964      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                      77.0000
  PRESSURE DROP                         PSI                     5.00000
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000


                       ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                    77.000
  OUTLET PRESSURE       PSIA                                 19.130
  HEAT DUTY             BTU/HR                              -95184.
  OUTLET VAPOR FRACTION                                      0.24904E-01
  PRESSURE-DROP CORRELATION PARAMETER                        0.44418E+07


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)          K(I)
     OXYGEN           0.23232E-01   0.15161E-03   0.92690       6113.7
     NITROGEN         0.77185E-04   0.77871E-07   0.30962E-02   39762.
     AMMONIA          0.25394E-04   0.25413E-04   0.24663E-04   0.97048
     WATER            0.81997       0.84003       0.34177E-01   0.40685E-
01
     CARBO-01         0.92621E-03   0.93021E-04   0.33549E-01    360.67
     METDIAMI         0.17093E-06   0.17500E-06   0.11966E-07   0.68384E-
01
     METHYLPI         0.15593E-02   0.15896E-02   0.37350E-03   0.23498
     3-MET-01         0.13893E-02   0.14198E-02   0.19710E-03   0.13883
     NICOT-01         0.15283       0.15669       0.16856E-02   0.10758E-
01
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                   03/27/2013  PAGE 44
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  HX-203   MODEL: HEATER
------------------------------
  INLET STREAM:          S-212
  OUTLET STREAM:         S-213
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           154.898         154.898          0.00000
      MASS(LB/HR   )           5795.22         5795.22          0.00000
      ENTHALPY(BTU/HR  )      -0.166063E+08   -0.166135E+08    0.434383E-03

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            7.43964      LB/HR
   PRODUCT STREAMS CO2E         7.43964      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                           77.0000
  PRESSURE DROP                      PSI                         10.0000
  MAXIMUM NO. ITERATIONS                                         30
  CONVERGENCE TOLERANCE                                           0.000100000


                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                     77.000
  OUTLET PRESSURE       PSIA                                  19.730
  HEAT DUTY             BTU/HR                               -7216.6
  OUTLET VAPOR FRACTION                                       0.29258E-01
  PRESSURE-DROP CORRELATION PARAMETER                         0.10240E+08
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                   03/27/2013  PAGE 45
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  HX-203   MODEL: HEATER (CONTINUED)

  V-L PHASE EQUILIBRIUM :

     COMP              F(I)          X(I)          Y(I)            K(I)
     OXYGEN          0.27373E-01   0.72082E-04   0.93318          12947.
     NITROGEN        0.90944E-04   0.27570E-07   0.31074E-02
0.11272E+06
     AMMONIA         0.29921E-04   0.29577E-04   0.41360E-04      1.3984
     WATER           0.78787       0.81092       0.23215E-01    0.28627E-
01
     CARBO-01        0.10913E-02   0.52879E-04   0.35546E-01      672.24
     NIACINAM        0.17827       0.18364       0.28002E-06    0.15249E-
05
     METDIAMI        0.20141E-06   0.20077E-06   0.22263E-06      1.1091
     METHYLPI        0.18373E-02   0.17891E-02   0.34339E-02      1.9195
     3-MET-01        0.16370E-02   0.16468E-02   0.13118E-02    0.79667
     NICOT-01        0.18007E-02   0.18501E-02   0.16287E-03    0.88047E-
01

BLOCK:  HX-204   MODEL: HEATER
------------------------------
  INLET STREAM:          S-219
  OUTLET STREAM:         S-220
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           154.898         154.898          0.00000
      MASS(LB/HR   )           5795.22         5795.22          0.00000
      ENTHALPY(BTU/HR  )      -0.166071E+08   -0.166135E+08    0.388764E-03

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            7.43964      LB/HR
   PRODUCT STREAMS CO2E         7.43964      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                           77.0000
  PRESSURE DROP                      PSI                         10.0000
  MAXIMUM NO. ITERATIONS                                         30
  CONVERGENCE TOLERANCE                                           0.000100000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 46
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  HX-204   MODEL: HEATER (CONTINUED)

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                     77.000
  OUTLET PRESSURE       PSIA                                  20.230
  HEAT DUTY             BTU/HR                               -6458.7
  OUTLET VAPOR FRACTION                                       0.29234E-01
  PRESSURE-DROP CORRELATION PARAMETER                         0.10459E+08


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)           K(I)
     OXYGEN           0.27373E-01   0.73961E-04   0.93387        12627.
     NITROGEN         0.90944E-04   0.28291E-07   0.31099E-02
0.10993E+06
     AMMONIA          0.29921E-04   0.29606E-04   0.40386E-04    1.3641
     WATER            0.78787       0.81092       0.22648E-01   0.27928E-
01
     CARBO-01         0.10913E-02   0.54188E-04   0.35531E-01    655.72
     NIACINAM         0.17827       0.18364       0.27336E-06   0.14887E-
05
     METDIAMI         0.20141E-06   0.20092E-06   0.21748E-06    1.0826
     METHYLPI         0.18373E-02   0.17915E-02   0.33557E-02    1.8733
     3-MET-01         0.16370E-02   0.16477E-02   0.12809E-02   0.77747
     NICOT-01         0.18007E-02   0.18501E-02   0.15898E-03   0.85938E-
01

BLOCK:  HX-205   MODEL: HEATER
------------------------------
  INLET STREAM:          S-226
  OUTLET STREAM:         S-227
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                     IN             OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            154.898         154.898         0.00000
      MASS(LB/HR   )            5795.22         5795.22         0.00000
      ENTHALPY(BTU/HR  )     -0.166049E+08   -0.167907E+08   0.110659E-01

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             7.43964      LB/HR
   PRODUCT STREAMS CO2E          7.43964      LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 47
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  HX-205   MODEL: HEATER (CONTINUED)

                          ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE              F                         32.0000
  PRESSURE DROP                      PSI                       10.0000
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000


                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                     32.000
  OUTLET PRESSURE       PSIA                                  27.730
  HEAT DUTY             BTU/HR                               -0.18580E+06
  OUTLET VAPOR FRACTION                                       0.28529E-01
  PRESSURE-DROP CORRELATION PARAMETER                         0.14353E+08


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)           K(I)
     OXYGEN           0.27373E-01   0.81854E-04   0.95669        11688.
     NITROGEN         0.90944E-04   0.23462E-07   0.31870E-02
0.13584E+06
     AMMONIA          0.29921E-04   0.30520E-04   0.95389E-05   0.31255
     WATER            0.78787       0.81092       0.31447E-02   0.38780E-
02
     CARBO-01         0.10913E-02   0.93331E-04   0.35075E-01    375.82
     NIACINAM         0.17827       0.18350       0.12063E-07   0.65739E-
07
     METDIAMI         0.20141E-06   0.20525E-06   0.70681E-07   0.34440
     METHYLPI         0.18373E-02   0.18496E-02   0.14171E-02   0.76622
     3-MET-01         0.16370E-02   0.16722E-02   0.43884E-03   0.26245
     NICOT-01         0.18007E-02   0.18524E-02   0.39603E-04   0.21381E-
01

BLOCK:  HX-206   MODEL: HEATER
------------------------------
  INLET STREAM:          S-230
  OUTLET STREAM:         S-231
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                     IN             OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            150.449         150.449         0.00000
      MASS(LB/HR   )            5650.33         5650.33         0.00000
      ENTHALPY(BTU/HR  )     -0.167575E+08   -0.165340E+08   -0.133365E-01
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                    03/27/2013  PAGE 48
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  HX-206   MODEL: HEATER (CONTINUED)

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.346806      LB/HR
   PRODUCT STREAMS CO2E        0.346806      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                           90.0000
  PRESSURE DROP                      PSI                         10.0000
  MAXIMUM NO. ITERATIONS                                         30
  CONVERGENCE TOLERANCE                                           0.000100000


                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                    90.000
  OUTLET PRESSURE       PSIA                                 35.000
  HEAT DUTY             BTU/HR                               0.22349E+06
  OUTLET VAPOR FRACTION                                      0.0000
  PRESSURE-DROP CORRELATION PARAMETER                        0.16232E+09


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)          K(I)
     OXYGEN           0.44082E-04   0.44082E-04   0.86921        6855.5
     NITROGEN         0.12611E-07   0.12611E-07   0.20087E-02    55375.
     AMMONIA          0.30292E-04   0.30292E-04   0.92705E-04    1.0640
     WATER            0.81100       0.81100       0.58025E-01   0.24875E-
01
     CARBO-01         0.52378E-04   0.52378E-04   0.60843E-01    403.86
     NIACINAM         0.18354       0.18354       0.96743E-06   0.18326E-
05
     METDIAMI         0.20363E-06   0.20363E-06   0.46919E-06   0.80108
     METHYLPI         0.18171E-02   0.18171E-02   0.67651E-02    1.2944
     3-MET-01         0.16620E-02   0.16620E-02   0.26899E-02   0.56269
     NICOT-01         0.18518E-02   0.18518E-02   0.36058E-03   0.67697E-
01

BLOCK:  HX-301   MODEL: HEATER
------------------------------
  INLET STREAM:          S-301
  OUTLET STREAM:         S-302
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                    03/27/2013  PAGE 49
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  HX-301   MODEL: HEATER (CONTINUED)

                   ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1259.04          1259.04          0.00000
      MASS(LB/HR   )           25618.8          25618.8          0.00000
      ENTHALPY(BTU/HR  )     -0.155047E+09   -0.153808E+09   -0.798587E-02

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.365887      LB/HR
   PRODUCT STREAMS CO2E        0.365887      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                           77.0000
  PRESSURE DROP                      PSI                         10.0000
  MAXIMUM NO. ITERATIONS                                         30
  CONVERGENCE TOLERANCE                                           0.000100000


                        ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                    77.000
  OUTLET PRESSURE       PSIA                                 25.000
  HEAT DUTY             BTU/HR                               0.12382E+07
  OUTLET VAPOR FRACTION                                      0.26201E-03
  PRESSURE-DROP CORRELATION PARAMETER                        0.60526E+07


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)          K(I)
     OXYGEN           0.52843E-05   0.14334E-06   0.19622E-01
0.13689E+06
     NITROGEN         0.59356E-07   0.72672E-10   0.22627E-03
0.31135E+07
     AMMONIA          0.24995E-02   0.24998E-02   0.12031E-02   0.48129
     WATER            0.97492       0.97517       0.12805E-01   0.13131E-
01
     CARBO-01         0.66033E-05   0.17511E-05   0.18521E-01    10577.
     NIACINAM         0.21932E-01   0.21938E-01   0.74823E-05   0.34107E-
03
     METDIAMI         0.24333E-07   0.79722E-09   0.89830E-04
0.11268E+06
     METHYLPI         0.21713E-03   0.53865E-04   0.62321        11570.
     3-MET-01         0.19874E-03   0.14939E-03   0.18851        1261.9
     NICOT-01         0.22129E-03   0.18575E-03   0.13581        731.15
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 50
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  HX-302   MODEL: HEATER
------------------------------
  INLET STREAM:          S-306
  OUTLET STREAM:         S-307
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          1259.04          1259.04         0.00000
      MASS(LB/HR   )          25618.8          25618.8         0.00000
      ENTHALPY(BTU/HR  )    -0.153806E+09   -0.124883E+09   -0.188044

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E          0.365887      LB/HR
   PRODUCT STREAMS CO2E       0.365887      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                        392.000
  PRESSURE DROP                      PSI                       10.0000
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000


                        ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                  392.00
  OUTLET PRESSURE       PSIA                               29.946
  HEAT DUTY             BTU/HR                            0.28922E+08
  OUTLET VAPOR FRACTION                                    1.0000
  PRESSURE-DROP CORRELATION PARAMETER                      14256.
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 51
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  HX-302   MODEL: HEATER (CONTINUED)

  V-L PHASE EQUILIBRIUM :

     COMP             F(I)           X(I)           Y(I)           K(I)
     OXYGEN         0.52843E-05    0.52701E-08    0.52843E-05     1085.6
     NITROGEN       0.59356E-07    0.27806E-10    0.59356E-07     2311.2
     AMMONIA        0.24995E-02    0.32318E-04    0.24995E-02     83.735
     WATER          0.97492        0.10980        0.97492         9.6137
     CARBO-01       0.66033E-05    0.23249E-07    0.66033E-05     307.51
     NIACINAM       0.21932E-01    0.88975        0.21932E-01    0.26688E-
01
     METDIAMI       0.24333E-07    0.13252E-07    0.24333E-07     1.9880
     METHYLPI       0.21713E-03    0.78107E-04    0.21713E-03     3.0099
     3-MET-01       0.19874E-03    0.68560E-04    0.19874E-03     3.1385
     NICOT-01       0.22129E-03    0.27092E-03    0.22129E-03    0.88435

BLOCK:  HX-303   MODEL: HEATER
------------------------------
  INLET STREAM:          S-308
  OUTLET STREAM:         S-309
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          1.10231          1.10231         0.00000
      MASS(LB/HR   )          30.8796          30.8796         0.00000
      ENTHALPY(BTU/HR  )     -5.93636          2425.28        -1.00245

                   ***  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                        392.000
  PRESSURE DROP                      PSI                       10.0000
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                    03/27/2013  PAGE 52
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  HX-303   MODEL: HEATER (CONTINUED)

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                  392.00
  OUTLET PRESSURE       PSIA                               19.501
  HEAT DUTY             BTU/HR                             2431.2
  OUTLET VAPOR FRACTION                                    1.0000
  PRESSURE-DROP CORRELATION PARAMETER                     0.61542E+10


  V-L PHASE EQUILIBRIUM :

     COMP           F(I)          X(I)          Y(I)           K(I)
     NITROGEN       1.0000        1.0000        1.0000         MISSING

BLOCK:  HX-304A  MODEL: HEATER
------------------------------
  INLET STREAM:          S-311
  OUTLET STREAM:         S-312A
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN             OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1241.79        1241.79         0.00000
      MASS(LB/HR   )           22481.2        22481.2         0.00000
      ENTHALPY(BTU/HR  )     -0.119198E+09  -0.152060E+09    0.216115

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            3.46806      LB/HR
   PRODUCT STREAMS CO2E         3.46806      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                       100.000
  PRESSURE DROP                      PSI                       5.00000
  MAXIMUM NO. ITERATIONS                                     30
  CONVERGENCE TOLERANCE                                        0.000100000
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                    03/27/2013  PAGE 53
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  HX-304A  MODEL: HEATER (CONTINUED)

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                        100.00
  OUTLET PRESSURE       PSIA                                     63.008
  HEAT DUTY             BTU/HR                                 -0.32862E+08
  OUTLET VAPOR FRACTION                                          0.91074E-02
  PRESSURE-DROP CORRELATION PARAMETER                            11710.


  V-L PHASE EQUILIBRIUM :

     COMP           F(I)          X(I)          Y(I)           K(I)
     OXYGEN         0.53407E-04   0.60207E-07   0.58576E-02    97291.
     NITROGEN       0.88768E-02   0.41595E-06   0.97464
0.23431E+07
     AMMONIA        0.25354E-02   0.25504E-02   0.89734E-03    0.35184
     WATER          0.98847       0.99745       0.11718E-01    0.11748E-
01
     CARBO-01       0.63459E-04   0.70059E-06   0.68916E-02    9836.8

BLOCK:  HX-304B  MODEL: HEATER
------------------------------
  INLET STREAM:          S-312A
  OUTLET STREAM:         S-312
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN             OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1241.79        1241.79         0.00000
      MASS(LB/HR   )           22481.2        22481.2         0.00000
      ENTHALPY(BTU/HR  )     -0.152060E+09  -0.153812E+09    0.113920E-01

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            3.46806      LB/HR
   PRODUCT STREAMS CO2E         3.46806      LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 54
                              NIACIN PRODUCTION
                              U-O-S BLOCK SECTION

 BLOCK:  HX-304B  MODEL: HEATER (CONTINUED)

                          ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE                 F                        32.0000
   PRESSURE DROP                         PSI                       5.00000
   MAXIMUM NO. ITERATIONS                                         30
   CONVERGENCE TOLERANCE                                           0.000100000


                           ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                     32.000
   OUTLET PRESSURE       PSIA                                  58.008
   HEAT DUTY             BTU/HR                               -0.17522E+07
   OUTLET VAPOR FRACTION                                       0.90036E-02
   PRESSURE-DROP CORRELATION PARAMETER                         0.11032E+07


   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)           K(I)
      OXYGEN          0.53407E-04    0.19036E-07    0.59297E-02
0.31150E+06
      NITROGEN        0.88768E-02    0.65762E-07    0.98592
0.14992E+08
      AMMONIA         0.25354E-02    0.25571E-02    0.14363E-03    0.56168E-
01
      WATER           0.98847        0.99744        0.10054E-02    0.10080E-
02
      CARBO-01        0.63459E-04    0.39145E-06    0.70051E-02     17895.

 BLOCK:  M-101    MODEL: MIXER
 -----------------------------
   INLET STREAMS:         S-102       S-109
   OUTLET STREAM:         S-103
   PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                      ***  MASS AND ENERGY BALANCE  ***
                                     IN              OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            28.7464         28.7464         0.00000
       MASS(LB/HR   )            3340.34         3340.34         0.00000
       ENTHALPY(BTU/HR  )      -0.204694E+07   -0.204694E+07   -0.494793E-13
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 55
                               NIACIN PRODUCTION
                               U-O-S BLOCK SECTION

  BLOCK:  M-101    MODEL: MIXER (CONTINUED)

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

  BLOCK:  M-201    MODEL: MIXER
  -----------------------------
    INLET STREAMS:         S-119       S-202
    OUTLET STREAM:         S-203A
    PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                       ***  MASS AND ENERGY BALANCE  ***
                                      IN              OUT        RELATIVE DIFF.
     TOTAL BALANCE
        MOLE(LBMOL/HR)            122.233         122.233          0.00000
        MASS(LB/HR   )            4313.94         4313.94          0.210827E-15
        ENTHALPY(BTU/HR  )      -0.773225E+07   -0.773225E+07    0.183524E-06

                       ***  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      FLASH
    MAXIMUM NO. ITERATIONS                                        30
    CONVERGENCE TOLERANCE                                          0.000100000
    OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 56
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  M-202    MODEL: MIXER
-----------------------------
  INLET STREAMS:         S-209       S-211
  OUTLET STREAM:         S-212
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           154.898         154.898        0.00000
      MASS(LB/HR   )           5795.22         5795.22      -0.313878E-15
      ENTHALPY(BTU/HR  )     -0.166063E+08   -0.166063E+08    0.476387E-09

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            7.43964      LB/HR
   PRODUCT STREAMS CO2E         7.43964      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:  M-203    MODEL: MIXER
-----------------------------
  INLET STREAMS:         S-216       S-218
  OUTLET STREAM:         S-219
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           154.898         154.898        0.00000
      MASS(LB/HR   )           5795.22         5795.22      -0.156939E-15
      ENTHALPY(BTU/HR  )     -0.166071E+08   -0.166071E+08    0.470319E-09
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 57
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  M-203    MODEL: MIXER (CONTINUED)

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            7.43964      LB/HR
   PRODUCT STREAMS CO2E         7.43964      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:  M-204    MODEL: MIXER
-----------------------------
  INLET STREAMS:         S-223       S-225
  OUTLET STREAM:         S-226
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT       RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           154.898         154.898        0.00000
      MASS(LB/HR   )           5795.22         5795.22      -0.156939E-15
      ENTHALPY(BTU/HR  )     -0.166049E+08   -0.166049E+08    0.217430E-08

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            7.43964      LB/HR
   PRODUCT STREAMS CO2E         7.43964      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
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                    03/27/2013  PAGE 58
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  M-301    MODEL: MIXER
-----------------------------
  INLET STREAMS:         S-231       S-318       S-201
  OUTLET STREAM:         S-301
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1259.04         1259.04        0.00000
      MASS(LB/HR   )           25618.8         25618.8       0.426013E-15
      ENTHALPY(BTU/HR  )     -0.155047E+09   -0.155047E+09   -0.592023E-13

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E          0.365887      LB/HR
   PRODUCT STREAMS CO2E       0.365887      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                                    50
  CONVERGENCE TOLERANCE                                      0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  N-301    MODEL: RSTOIC
------------------------------
  INLET STREAMS:         S-304       S-303
  OUTLET STREAM:         S-305
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                              IN          OUT       GENERATION   RELATIVE
DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)         1259.04       1259.04     -0.165655E-15 -0.361187E-
15
  MASS(LB/HR   )         25618.8       25618.8                  -0.426013E-
15
  ENTHALPY(BTU/HR  )   -0.153808E+09 -0.153810E+09               0.969732E-
05
```

```
ASPEN PLUS   PLAT: WIN32    VER: 25.0                    03/27/2013  PAGE 59
                            NIACIN PRODUCTION
                            U-O-S BLOCK SECTION

BLOCK:  N-301    MODEL: RSTOIC (CONTINUED)

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E          0.365887      LB/HR
   PRODUCT STREAMS CO2E       0.365887      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  ***
  STOICHIOMETRY MATRIX:

   REACTION #   1:
    SUBSTREAM MIXED    :
    WATER     -1.00    NIACINAM  -1.00    AMMONICO   1.00
    SUBSTREAM CIPSD    :
    NO PARTICIPATING COMPONENTS

   REACTION #   2:
    SUBSTREAM MIXED    :
    WATER      1.00    NIACINAM   1.00    AMMONICO  -1.00
    SUBSTREAM CIPSD    :
    NO PARTICIPATING COMPONENTS

  REACTION CONVERSION SPECS: NUMBER=    2
    REACTION #   1:
    SUBSTREAM:MIXED    KEY COMP:NIACINAM CONV FRAC:  1.000
    REACTION #   2:
    SUBSTREAM:MIXED    KEY COMP:AMMONICO CONV FRAC:  1.000


  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE F                                   77.0000
  PRESSURE DROP          PSI                                 5.00000
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                      0.000100000
  SERIES REACTIONS
  GENERATE COMBUSTION REACTIONS FOR FEED SPECIES           NO
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                        03/27/2013  PAGE 60
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  N-301    MODEL: RSTOIC (CONTINUED)

                       ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                  77.000
  OUTLET PRESSURE       PSIA                               15.000
  HEAT DUTY             BTU/HR                            -1491.5
  VAPOR FRACTION                                          0.35328E-03


  REACTION EXTENTS:

     REACTION          REACTION
     NUMBER            EXTENT
                       LBMOL/HR
     1                  27.614
     2                  27.614

  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     OXYGEN          0.52843E-05    0.60926E-07    0.14785E-01
0.24268E+06
     NITROGEN        0.59356E-07    0.30314E-10    0.16793E-03
0.55395E+07
     AMMONIA         0.24995E-02    0.24996E-02    0.20677E-02    0.82721
     WATER           0.97492        0.97526        0.21653E-01    0.22202E-
01
     CARBO-01        0.66033E-05    0.88085E-06    0.16199E-01     18390.
     NIACINAM        0.21932E-01    0.21940E-01    0.11239E-04    0.51228E-
03
     METDIAMI        0.24333E-07    0.39200E-09    0.67768E-04
0.17288E+06
     METHYLPI        0.21713E-03    0.29085E-04    0.53232         18302.
     3-MET-01        0.19874E-03    0.11620E-03    0.23374         2011.5
     NICOT-01        0.22129E-03    0.15811E-03    0.17899         1132.0

BLOCK:  P-101    MODEL: PUMP
----------------------------
  INLET STREAM:          S-101
  OUTLET STREAM:         S-102
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                        03/27/2013  PAGE 61
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  P-101    MODEL: PUMP (CONTINUED)

                       ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT          RELATIVE DIFF.
  TOTAL BALANCE
     MOLE(LBMOL/HR)             28.4590         28.4590         0.00000
     MASS(LB/HR    )            3306.93         3306.93         0.00000
     ENTHALPY(BTU/HR  )      -0.203415E+07   -0.203317E+07   -0.481539E-03

                       ***  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                                      43.5113
  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                              53.9515
  PRESSURE CHANGE  PSI                                       29.0075
  NPSH AVAILABLE   FT-LBF/LB                                 34.0618
  FLUID POWER  HP                                             0.11382
  BRAKE POWER  HP                                             0.38497
  ELECTRICITY  KW                                             0.28707
  PUMP EFFICIENCY USED                                        0.29566
  NET WORK REQUIRED  HP                                       0.38497
  HEAD DEVELOPED FT-LBF/LB                                   68.1477

BLOCK:  P-102    MODEL: PUMP
----------------------------
  INLET STREAM:          S-108
  OUTLET STREAM:         S-109
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

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

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                      03/27/2013  PAGE 62
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  P-102    MODEL: PUMP (CONTINUED)
   TOTAL BALANCE
      MOLE(LBMOL/HR)          0.287465        0.287465        0.00000
      MASS(LB/HR   )          33.4028         33.4028         0.00000
      ENTHALPY(BTU/HR  )     -13787.0        -13777.3        -0.704878E-03

                 ***  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                                  43.5113
   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                           0.67609
   PRESSURE CHANGE  PSI                                   22.9654
   NPSH AVAILABLE   FT-LBF/LB                              0.0
   FLUID POWER  HP                                         0.0011292
   BRAKE POWER  HP                                         0.0038193
   ELECTRICITY  KW                                         0.0028481
   PUMP EFFICIENCY USED                                    0.29566
   NET WORK REQUIRED  HP                                   0.0038193
   HEAD DEVELOPED FT-LBF/LB                               66.9359

BLOCK:  P-103    MODEL: PUMP
----------------------------
  INLET STREAM:          S-116
  OUTLET STREAM:         S-117
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                 ***  MASS AND ENERGY BALANCE  ***
                                  IN             OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          66.6101         66.6101         0.00000
      MASS(LB/HR   )          1200.00         1200.00         0.00000
      ENTHALPY(BTU/HR  )     -0.825936E+07   -0.825747E+07   -0.228763E-03
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                      03/27/2013  PAGE 63
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  P-103    MODEL: PUMP (CONTINUED)

                 ***  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                                 170.000
   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                          19.4761
   PRESSURE CHANGE  PSI                                  155.000
   NPSH AVAILABLE   FT-LBF/LB                             33.8472
   FLUID POWER  HP                                         0.21955
   BRAKE POWER  HP                                         0.74258
   ELECTRICITY  KW                                         0.55374
   PUMP EFFICIENCY USED                                    0.29566
   NET WORK REQUIRED  HP                                   0.74258
   HEAD DEVELOPED FT-LBF/LB                              362.255

BLOCK:  P-201    MODEL: PUMP
----------------------------
  INLET STREAM:          S-210
  OUTLET STREAM:         S-211
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                 ***  MASS AND ENERGY BALANCE  ***
                                  IN             OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          150.317         150.317         0.00000
      MASS(LB/HR   )          5646.78         5646.78         0.00000
      ENTHALPY(BTU/HR  )     -0.165700E+08   -0.165693E+08   -0.432513E-04

                 ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.261936     LB/HR
   PRODUCT STREAMS CO2E         0.261936     LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 64
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  P-201    MODEL: PUMP (CONTINUED)

                       ***  INPUT DATA  ***
   PRESSURE CHANGE  PSI                                  15.0000
   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                         76.3381
   PRESSURE CHANGE  PSI                                  15.0000
   NPSH AVAILABLE   FT-LBF/LB                            -0.0029243
   FLUID POWER  HP                                        0.083278
   BRAKE POWER  HP                                        0.28167
   ELECTRICITY  KW                                        0.21004
   PUMP EFFICIENCY USED                                   0.29566
   NET WORK REQUIRED  HP                                  0.28167
   HEAD DEVELOPED FT-LBF/LB                              29.2008
   NEGATIVE NPSH MAY BE DUE TO VAPOR IN THE FEED OR UNACCOUNTED SUCTION HEAD.

BLOCK:  P-202    MODEL: PUMP
----------------------------
  INLET STREAM:         S-217
  OUTLET STREAM:        S-218
  PROPERTY OPTION SET:  RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           150.324         150.324         0.00000
      MASS(LB/HR   )           5646.98         5646.98         0.161059E-15
      ENTHALPY(BTU/HR  )     -0.165707E+08   -0.165700E+08   -0.432514E-04

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.270835      LB/HR
   PRODUCT STREAMS CO2E        0.270835      LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 65
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  P-202    MODEL: PUMP (CONTINUED)

                       ***  INPUT DATA  ***
   PRESSURE CHANGE  PSI                                  15.0000
   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                         76.3413
   PRESSURE CHANGE  PSI                                  15.0000
   NPSH AVAILABLE   FT-LBF/LB                             0.0
   FLUID POWER  HP                                        0.083281
   BRAKE POWER  HP                                        0.28168
   ELECTRICITY  KW                                        0.21005
   PUMP EFFICIENCY USED                                   0.29566
   NET WORK REQUIRED  HP                                  0.28168
   HEAD DEVELOPED FT-LBF/LB                              29.2010

BLOCK:  P-203    MODEL: PUMP
----------------------------
  INLET STREAM:         S-224
  OUTLET STREAM:        S-225
  PROPERTY OPTION SET:  RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           150.329         150.329         0.00000
      MASS(LB/HR   )           5647.16         5647.16         0.00000
      ENTHALPY(BTU/HR  )     -0.165713E+08   -0.165698E+08   -0.865050E-04

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.279711      LB/HR
   PRODUCT STREAMS CO2E        0.279711      LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000      LB/HR
   UTILITIES CO2E PRODUCTION    0.00000      LB/HR
   TOTAL CO2E PRODUCTION        0.00000      LB/HR
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 66
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  P-203    MODEL: PUMP (CONTINUED)

                      ***  INPUT DATA  ***
   PRESSURE CHANGE  PSI                                    30.0000
   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                           76.3443
   PRESSURE CHANGE  PSI                                    30.0000
   NPSH AVAILABLE   FT-LBF/LB                               0.0
   FLUID POWER  HP                                          0.16657
   BRAKE POWER  HP                                          0.56339
   ELECTRICITY  KW                                          0.42012
   PUMP EFFICIENCY USED                                     0.29566
   NET WORK REQUIRED  HP                                    0.56339
   HEAD DEVELOPED FT-LBF/LB                                58.4023

BLOCK:  P-204    MODEL: PUMP
----------------------------
  INLET STREAM:          S-229
  OUTLET STREAM:         S-230
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           150.449         150.449          0.00000
      MASS(LB/HR   )           5650.33         5650.33       -0.321926E-15
      ENTHALPY(BTU/HR  )    -0.167589E+08   -0.167575E+08   -0.838361E-04

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.346806       LB/HR
   PRODUCT STREAMS CO2E        0.346806       LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000       LB/HR
   UTILITIES CO2E PRODUCTION    0.00000       LB/HR
   TOTAL CO2E PRODUCTION        0.00000       LB/HR
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 67
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  P-204    MODEL: PUMP (CONTINUED)

                      ***  INPUT DATA  ***
   PRESSURE CHANGE  PSI                                    30.0000
   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                           74.8273
   PRESSURE CHANGE  PSI                                    30.0000
   NPSH AVAILABLE   FT-LBF/LB                              -0.0035963
   FLUID POWER  HP                                          0.16326
   BRAKE POWER  HP                                          0.55219
   ELECTRICITY  KW                                          0.41177
   PUMP EFFICIENCY USED                                     0.29566
   NET WORK REQUIRED  HP                                    0.55219
   HEAD DEVELOPED FT-LBF/LB                                57.2098
   NEGATIVE NPSH MAY BE DUE TO VAPOR IN THE FEED OR UNACCOUNTED SUCTION HEAD.

BLOCK:  P-301    MODEL: PUMP
----------------------------
  INLET STREAM:          S-305
  OUTLET STREAM:         S-306
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1259.04         1259.04          0.00000
      MASS(LB/HR   )           25618.8         25618.8          0.00000
      ENTHALPY(BTU/HR  )    -0.153810E+09   -0.153806E+09   -0.273118E-04

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.365887       LB/HR
   PRODUCT STREAMS CO2E        0.365887       LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000       LB/HR
   UTILITIES CO2E PRODUCTION    0.00000       LB/HR
   TOTAL CO2E PRODUCTION        0.00000       LB/HR
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                        03/27/2013  PAGE 68
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  P-301    MODEL: PUMP (CONTINUED)

                       ***  INPUT DATA  ***
   PRESSURE CHANGE  PSI                                          24.9465
   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                                400.442
   PRESSURE CHANGE  PSI                                          24.9465
   NPSH AVAILABLE   FT-LBF/LB                                  -213.682
   FLUID POWER  HP                                                0.72652
   BRAKE POWER  HP                                                1.65276
   ELECTRICITY  KW                                                1.23247
   PUMP EFFICIENCY USED                                           0.43958
   NET WORK REQUIRED  HP                                          1.65276
   HEAD DEVELOPED FT-LBF/LB                                      56.1504
   NEGATIVE NPSH MAY BE DUE TO VAPOR IN THE FEED OR UNACCOUNTED SUCTION HEAD.

BLOCK:  R-101    MODEL: RSTOIC
------------------------------
  INLET STREAM:          S-105
  OUTLET STREAM:         S-106
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                             IN           OUT       GENERATION   RELATIVE
DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)         28.7464       57.2054       28.4590       0.00000
  MASS(LB/HR   )         3340.34       3340.35                    -0.477106E-
05
  ENTHALPY(BTU/HR  )    -522590.      -974645.                     0.463815

                   ***  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  ***
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                        03/27/2013  PAGE 69
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  R-101    MODEL: RSTOIC (CONTINUED)
  STOICHIOMETRY MATRIX:

   REACTION #   1:
    SUBSTREAM MIXED    :
    AMMONIA     1.00    METDIAMI  -1.00    METHYLPI   1.00
    SUBSTREAM CIPSD    :
    NO PARTICIPATING COMPONENTS


  REACTION CONVERSION SPECS: NUMBER=    1
    REACTION #   1:
    SUBSTREAM:MIXED    KEY COMP:METDIAMI CONV FRAC: 0.9900



  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE F                                       581.000
  PRESSURE DROP          PSI                                      0.87023
  MAXIMUM NO. ITERATIONS                                        30
  CONVERGENCE TOLERANCE                                           0.000100000
  SIMULTANEOUS REACTIONS
  GENERATE COMBUSTION REACTIONS FOR FEED SPECIES               NO

                        ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                         581.00
  OUTLET PRESSURE       PSIA                                      71.649
  HEAT DUTY             BTU/HR                                   -0.45205E+06
  VAPOR FRACTION                                                   1.0000


  REACTION EXTENTS:

     REACTION           REACTION
     NUMBER             EXTENT
                        LBMOL/HR
     1                   28.459

  V-L PHASE EQUILIBRIUM :

     COMP               F(I)           X(I)           Y(I)           K(I)
     AMMONIA           0.49749        0.89068E-01    0.49749        27.859
     METDIAMI          0.50251E-02    0.13718E-01    0.50251E-02    1.8272
     METHYLPI          0.49749        0.89721        0.49749        2.7657

BLOCK:  R-102    MODEL: RSTOIC
------------------------------
  INLET STREAM:          S-111
  OUTLET STREAM:         S-112
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 70
                              NIACIN PRODUCTION
                              U-O-S BLOCK SECTION

 BLOCK:  R-102    MODEL: RSTOIC (CONTINUED)

                    ***  MASS AND ENERGY BALANCE  ***
                                IN           OUT       GENERATION   RELATIVE
DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)         56.9179       141.441       84.5231       0.200944E-
15
   MASS(LB/HR   )         3306.95       3307.12                    -0.507751E-
04
   ENTHALPY(BTU/HR  )   -0.102115E+07  0.158151E+07                 -1.64568

                    ***  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  ***
   STOICHIOMETRY MATRIX:

    REACTION #   1:
     SUBSTREAM MIXED   :
     HYDROGEN   3.00    METHYLPI  -1.00    3-MET-01   1.00
     SUBSTREAM CIPSD   :
     NO PARTICIPATING COMPONENTS


   REACTION CONVERSION SPECS: NUMBER=    1
     REACTION #   1:
     SUBSTREAM:MIXED    KEY COMP:METHYLPI CONV FRAC: 0.9900



   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE F                                 554.000
   PRESSURE DROP          PSI                               20.3053
   MAXIMUM NO. ITERATIONS                                   30
   CONVERGENCE TOLERANCE                                     0.000100000
   SIMULTANEOUS REACTIONS
   GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO
```

```
 ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 71
                              NIACIN PRODUCTION
                              U-O-S BLOCK SECTION

 BLOCK:  R-102    MODEL: RSTOIC (CONTINUED)

                         ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                     554.00
   OUTLET PRESSURE       PSIA                                  42.214
   HEAT DUTY             BTU/HR                               0.26027E+07
   VAPOR FRACTION                                              1.0000


   REACTION EXTENTS:

      REACTION         REACTION
      NUMBER           EXTENT
                       LBMOL/HR
      1                 28.174

   V-L PHASE EQUILIBRIUM :

      COMP              F(I)          X(I)          Y(I)            K(I)
      HYDROGEN         0.59759       0.26382       0.59759         72.897
      AMMONIA          0.20121       0.19839       0.20121         36.044
      METDIAMI         0.22057E-06   0.84634E-06   0.22057E-06     8.2556
      METHYLPI         0.20121E-02   0.59577E-02   0.20121E-02     10.616
      3-MET-01         0.19920       0.53184       0.19920         11.738

 BLOCK:  R-201    MODEL: RSTOIC
 ------------------------------
   INLET STREAMS:          S-203        S-204
   OUTLET STREAM:          S-205
   PROPERTY OPTION SET:    RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                IN           OUT       GENERATION   RELATIVE
DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)          168.530       182.512       13.9814       0.00000
   MASS(LB/HR   )          5795.40       5795.40                   -0.156934E-
15
   ENTHALPY(BTU/HR  )   -0.513239E+07 -0.110133E+08                  0.533984
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                       03/27/2013  PAGE 72
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  R-201    MODEL: RSTOIC (CONTINUED)

                      ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             0.00000      LB/HR
   PRODUCT STREAMS CO2E          7.43964      LB/HR
   NET STREAMS CO2E PRODUCTION   7.43964      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         7.43964      LB/HR

                          ***  INPUT DATA  ***
  STOICHIOMETRY MATRIX:

   REACTION #   1:
    SUBSTREAM MIXED   :
    OXYGEN    -1.50    AMMONIA   -1.00    WATER      3.00    3-MET-01  -1.00
    NICOT-01   1.00
    SUBSTREAM CIPSD   :
    NO PARTICIPATING COMPONENTS

   REACTION #   2:
    SUBSTREAM MIXED   :
    OXYGEN    -15.5    NITROGEN   1.00    WATER      7.00    CARBO-01   12.0
    3-MET-01  -2.00
    SUBSTREAM CIPSD   :
    NO PARTICIPATING COMPONENTS


  REACTION CONVERSION SPECS: NUMBER=    2
    REACTION #   1:
    SUBSTREAM:MIXED    KEY COMP:3-MET-01 CONV FRAC: 0.9900
    REACTION #   2:
    SUBSTREAM:MIXED    KEY COMP:3-MET-01 CONV FRAC: 0.1000



  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE F                                 626.000
  PRESSURE DROP          PSI                                0.87023
  MAXIMUM NO. ITERATIONS                                   30
  CONVERGENCE TOLERANCE                                     0.000100000
  SERIES REACTIONS
  GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                       03/27/2013  PAGE 73
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  R-201    MODEL: RSTOIC (CONTINUED)

                             ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                 626.00
  OUTLET PRESSURE       PSIA                              29.130
  HEAT DUTY             BTU/HR                          -0.58809E+07
  VAPOR FRACTION                                          1.0000


  REACTION EXTENTS:

     REACTION          REACTION
     NUMBER            EXTENT
                       LBMOL/HR
     1                  27.892
     2                 0.14087E-01

  V-L PHASE EQUILIBRIUM :

     COMP              F(I)          X(I)          Y(I)          K(I)
     OXYGEN           0.23232E-01   0.61170E-02   0.23232E-01   91.523
     NITROGEN         0.77185E-04   0.17977E-04   0.77185E-04   103.47
     AMMONIA          0.25394E-04   0.12257E-04   0.25394E-04   49.930
     WATER            0.81997       0.55663       0.81997       35.499
     CARBO-01         0.92621E-03   0.32383E-03   0.92621E-03   68.927
     METDIAMI         0.17093E-06   0.46285E-06   0.17093E-06   8.8998
     METHYLPI         0.15593E-02   0.31949E-02   0.15593E-02   11.762
     3-MET-01         0.13893E-02   0.25124E-02   0.13893E-02   13.326
     NICOT-01         0.15283       0.43119       0.15283       8.5412

BLOCK:  R-202A   MODEL: RSTOIC
------------------------------
  INLET STREAM:          S-206
  OUTLET STREAM:         S-207
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

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

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 74
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  R-202A   MODEL: RSTOIC (CONTINUED)
  TOTAL BALANCE
  MOLE(LBMOL/HR)         182.512       154.898      -27.6135        0.00000
  MASS(LB/HR   )         5795.40       5795.22                      0.310661E-
04
  ENTHALPY(BTU/HR  )   -0.154853E+08 -0.166128E+08                  0.678664E-
01

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            7.43964      LB/HR
   PRODUCT STREAMS CO2E         7.43964      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  ***
  STOICHIOMETRY MATRIX:

   REACTION #   1:
    SUBSTREAM MIXED   :
    WATER     -1.00    NIACINAM   1.00    NICOT-01  -1.00
    SUBSTREAM CIPSD   :
    NO PARTICIPATING COMPONENTS


  REACTION CONVERSION SPECS: NUMBER=    1
    REACTION #   1:
    SUBSTREAM:MIXED    KEY COMP:NICOT-01 CONV FRAC: 0.9900



  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE F                                   77.0000
  PRESSURE DROP         PSI                                  4.40000
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                      0.000100000
  SIMULTANEOUS REACTIONS
  GENERATE COMBUSTION REACTIONS FOR FEED SPECIES           NO

                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                    77.000
  OUTLET PRESSURE       PSIA                                 14.730
  HEAT DUTY             BTU/HR                              -0.11279E+07
  VAPOR FRACTION                                             0.29574E-01
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 75
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  R-202A   MODEL: RSTOIC (CONTINUED)

  REACTION EXTENTS:

     REACTION         REACTION
     NUMBER           EXTENT
                      LBMOL/HR
     1                 27.614

  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)           K(I)
     OXYGEN          0.27373E-01   0.53288E-04   0.92383        17337.
     NITROGEN        0.90944E-04   0.20364E-07   0.30745E-02
0.15097E+06
     AMMONIA         0.29921E-04   0.29171E-04   0.54533E-04     1.8694
     WATER           0.78787       0.81094       0.31000E-01    0.38227E-
01
     CARBO-01        0.10913E-02   0.39595E-04   0.35602E-01     899.17
     NIACINAM        0.17827       0.18370       0.37163E-06    0.20230E-
05
     METDIAMI        0.20141E-06   0.19863E-06   0.29267E-06     1.4735
     METHYLPI        0.18373E-02   0.17565E-02   0.44868E-02     2.5543
     3-MET-01        0.16370E-02   0.16341E-02   0.17330E-02     1.0606
     NICOT-01        0.18007E-02   0.18490E-02   0.21638E-03    0.11702
BLOCK:  R-202B   MODEL: RSTOIC
-----------------------------
  INLET STREAM:          S-213
  OUTLET STREAM:         S-214
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                               IN          OUT       GENERATION   RELATIVE
DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)         154.898       154.898       0.00000       0.183486E-
15
  MASS(LB/HR   )         5795.22       5795.22                     0.156939E-
15
  ENTHALPY(BTU/HR  )   -0.166135E+08 -0.166129E+08                -0.357740E-
04

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            7.43964      LB/HR
   PRODUCT STREAMS CO2E         7.43964      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  ***
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                       03/27/2013  PAGE 76
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  R-202B   MODEL: RSTOIC (CONTINUED)
  STOICHIOMETRY MATRIX:

   REACTION #    1:
    SUBSTREAM MIXED   :
    WATER      1.00    NIACINAM  -1.00    NICOT-01   1.00
    SUBSTREAM CIPSD   :
    NO PARTICIPATING COMPONENTS

   REACTION #    2:
    SUBSTREAM MIXED   :
    WATER     -1.00    NIACINAM   1.00    NICOT-01  -1.00
    SUBSTREAM CIPSD   :
    NO PARTICIPATING COMPONENTS


  REACTION CONVERSION SPECS: NUMBER=    2
    REACTION #    1:
    SUBSTREAM:MIXED    KEY COMP:NIACINAM CONV FRAC:  1.000
    REACTION #    2:
    SUBSTREAM:MIXED    KEY COMP:NICOT-01 CONV FRAC: 0.9900



  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE F                                   77.0000
  PRESSURE DROP          PSI                                 4.50000
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                      0.000100000
  SERIES REACTIONS
  GENERATE COMBUSTION REACTIONS FOR FEED SPECIES           NO

                             ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                     77.000
  OUTLET PRESSURE       PSIA                                  15.230
  HEAT DUTY             BTU/HR                                594.33
  VAPOR FRACTION                                             0.29534E-01


  REACTION EXTENTS:

     REACTION          REACTION
     NUMBER            EXTENT
                       LBMOL/HR
     1                  27.614
     2                  27.614
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                       03/27/2013  PAGE 77
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  R-202B   MODEL: RSTOIC (CONTINUED)

  V-L PHASE EQUILIBRIUM :

     COMP               F(I)           X(I)           Y(I)           K(I)
     OXYGEN           0.27373E-01    0.55167E-04    0.92503        16768.
     NITROGEN         0.90944E-04    0.21084E-07    0.30786E-02
0.14602E+06
     AMMONIA          0.29921E-04    0.29224E-04    0.52848E-04    1.8084
     WATER            0.78787        0.81093        0.29991E-01    0.36984E-
01
     CARBO-01         0.10913E-02    0.40938E-04    0.35607E-01    869.77
     NIACINAM         0.17827        0.18369        0.35976E-06    0.19585E-
05
     METDIAMI         0.20141E-06    0.19890E-06    0.28368E-06    1.4262
     METHYLPI         0.18373E-02    0.17607E-02    0.43526E-02    2.4721
     3-MET-01         0.16370E-02    0.16357E-02    0.16789E-02    1.0264
     NICOT-01         0.18007E-02    0.18491E-02    0.20945E-03    0.11327

BLOCK:  R-202C   MODEL: RSTOIC
 ------------------------------
  INLET STREAM:          S-220
  OUTLET STREAM:         S-221
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                 IN          OUT      GENERATION   RELATIVE
DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)        154.898       154.898       0.00000      0.183486E-
15
  MASS(LB/HR   )        5795.22       5795.22                    0.156939E-
15
  ENTHALPY(BTU/HR  )   -0.166135E+08 -0.166130E+08              -0.334953E-
04

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            7.43964      LB/HR
   PRODUCT STREAMS CO2E         7.43964      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  ***
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 78
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  R-202C   MODEL: RSTOIC (CONTINUED)
  STOICHIOMETRY MATRIX:

   REACTION #   1:
    SUBSTREAM MIXED   :
    WATER      1.00    NIACINAM  -1.00    NICOT-01   1.00
    SUBSTREAM CIPSD   :
    NO PARTICIPATING COMPONENTS

   REACTION #   2:
    SUBSTREAM MIXED   :
    WATER     -1.00    NIACINAM   1.00    NICOT-01  -1.00
    SUBSTREAM CIPSD   :
    NO PARTICIPATING COMPONENTS


  REACTION CONVERSION SPECS: NUMBER=    2
    REACTION #   1:
    SUBSTREAM:MIXED    KEY COMP:NIACINAM CONV FRAC:  1.000
    REACTION #   2:
    SUBSTREAM:MIXED    KEY COMP:NICOT-01 CONV FRAC: 0.9900



  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE F                              77.0000
  PRESSURE DROP          PSI                            4.50000
  MAXIMUM NO. ITERATIONS                               30
  CONVERGENCE TOLERANCE                                 0.000100000
  SERIES REACTIONS
  GENERATE COMBUSTION REACTIONS FOR FEED SPECIES       NO

                        ***  RESULTS  ***
  OUTLET TEMPERATURE     F                              77.000
  OUTLET PRESSURE        PSIA                           15.730
  HEAT DUTY              BTU/HR                         556.47
  VAPOR FRACTION                                        0.29496E-01


  REACTION EXTENTS:

     REACTION          REACTION
     NUMBER            EXTENT
                       LBMOL/HR
     1                  27.614
     2                  27.614
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                     03/27/2013  PAGE 79
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  R-202C   MODEL: RSTOIC (CONTINUED)

  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     OXYGEN            0.27373E-01    0.57048E-04    0.92615        16235.
     NITROGEN          0.90944E-04    0.21805E-07    0.30826E-02
0.14137E+06
     AMMONIA           0.29921E-04    0.29273E-04    0.51264E-04    1.7512
     WATER             0.78787        0.81093        0.29047E-01    0.35819E-
01
     CARBO-01          0.10913E-02    0.42280E-04    0.35608E-01    842.24
     NIACINAM          0.17827        0.18369        0.34861E-06    0.18980E-
05
     METDIAMI          0.20141E-06    0.19916E-06    0.27520E-06    1.3820
     METHYLPI          0.18373E-02    0.17647E-02    0.42258E-02    2.3950
     3-MET-01          0.16370E-02    0.16373E-02    0.16278E-02    0.99434
     NICOT-01          0.18007E-02    0.18493E-02    0.20293E-03    0.10975

BLOCK:  SEP-201  MODEL: FLASH2
------------------------------
  INLET STREAM:          S-207
  OUTLET VAPOR STREAM:   S-208
  OUTLET LIQUID STREAM:  S-210
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                   ***  MASS AND ENERGY BALANCE  ***
                                  IN             OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           154.898         154.898      -0.183486E-15
      MASS(LB/HR   )           5795.22         5795.22       0.156939E-15
      ENTHALPY(BTU/HR  )     -0.166128E+08  -0.166128E+08    0.169258E-09

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           7.43964      LB/HR
   PRODUCT STREAMS CO2E        7.43964      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  PQ  FLASH
  PRESSURE DROP          PSI                            0.0
  SPECIFIED HEAT DUTY    BTU/HR                         0.0
  MAXIMUM NO. ITERATIONS                               30
  CONVERGENCE TOLERANCE                                 0.000100000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                  03/27/2013  PAGE 80
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  SEP-201  MODEL: FLASH2 (CONTINUED)

                        ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                   77.000
  OUTLET PRESSURE       PSIA                                14.730
  VAPOR FRACTION                                            0.29574E-01


  V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     OXYGEN          0.27373E-01   0.53288E-04   0.92383       17337.
     NITROGEN        0.90944E-04   0.20364E-07   0.30745E-02
0.15097E+06
     AMMONIA         0.29921E-04   0.29171E-04   0.54533E-04    1.8694
     WATER           0.78787       0.81094       0.31000E-01   0.38227E-
01
     CARBO-01        0.10913E-02   0.39595E-04   0.35602E-01    899.17
     NIACINAM        0.17827       0.18370       0.37163E-06   0.20230E-
05
     METDIAMI        0.20141E-06   0.19863E-06   0.29267E-06    1.4735
     METHYLPI        0.18373E-02   0.17565E-02   0.44868E-02    2.5543
     3-MET-01        0.16370E-02   0.16341E-02   0.17330E-02    1.0606
     NICOT-01        0.18007E-02   0.18490E-02   0.21638E-03   0.11702

BLOCK:  SEP-202  MODEL: FLASH2
------------------------------
  INLET STREAM:           S-214
  OUTLET VAPOR STREAM:    S-215
  OUTLET LIQUID STREAM:   S-217
  PROPERTY OPTION SET:    RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           154.898          154.898        0.00000
      MASS(LB/HR   )           5795.22          5795.22        0.00000
      ENTHALPY(BTU/HR  )    -0.166129E+08   -0.166129E+08    0.183965E-09

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            7.43964       LB/HR
   PRODUCT STREAMS CO2E         7.43964       LB/HR
   NET STREAMS CO2E PRODUCTION  0.00000       LB/HR
   UTILITIES CO2E PRODUCTION    0.00000       LB/HR
   TOTAL CO2E PRODUCTION        0.00000       LB/HR
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                  03/27/2013  PAGE 81
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  SEP-202  MODEL: FLASH2 (CONTINUED)

                        ***  INPUT DATA  ***
  TWO    PHASE  PQ  FLASH
  PRESSURE DROP         PSI                                  0.0
  SPECIFIED HEAT DUTY   BTU/HR                               0.0
  MAXIMUM NO. ITERATIONS                                    42
  CONVERGENCE TOLERANCE                                      0.000100000

                        ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                   77.000
  OUTLET PRESSURE       PSIA                                15.230
  VAPOR FRACTION                                            0.29534E-01


  V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     OXYGEN          0.27373E-01   0.55167E-04   0.92503       16768.
     NITROGEN        0.90944E-04   0.21084E-07   0.30786E-02
0.14602E+06
     AMMONIA         0.29921E-04   0.29224E-04   0.52848E-04    1.8084
     WATER           0.78787       0.81093       0.29991E-01   0.36984E-
01
     CARBO-01        0.10913E-02   0.40938E-04   0.35607E-01    869.77
     NIACINAM        0.17827       0.18369       0.35976E-06   0.19585E-
05
     METDIAMI        0.20141E-06   0.19890E-06   0.28368E-06    1.4262
     METHYLPI        0.18373E-02   0.17607E-02   0.43526E-02    2.4721
     3-MET-01        0.16370E-02   0.16357E-02   0.16789E-02    1.0264
     NICOT-01        0.18007E-02   0.18491E-02   0.20945E-03   0.11327

BLOCK:  SEP-203  MODEL: FLASH2
------------------------------
  INLET STREAM:          S-221
  OUTLET VAPOR STREAM:   S-222
  OUTLET LIQUID STREAM:  S-224
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           154.898          154.898        0.00000
      MASS(LB/HR   )           5795.22          5795.22        0.00000
      ENTHALPY(BTU/HR  )    -0.166130E+08   -0.166130E+08    0.199391E-09
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 82
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  SEP-203  MODEL: FLASH2 (CONTINUED)

                     *** CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             7.43964      LB/HR
   PRODUCT STREAMS CO2E          7.43964      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  PQ  FLASH
  PRESSURE DROP          PSI                                  0.0
  SPECIFIED HEAT DUTY   BTU/HR                                0.0
  MAXIMUM NO. ITERATIONS                                     30
  CONVERGENCE TOLERANCE                                       0.000100000

                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                     77.000
  OUTLET PRESSURE       PSIA                                  15.730
  VAPOR FRACTION                                              0.29496E-01


  V-L PHASE EQUILIBRIUM :

     COMP              F(I)          X(I)          Y(I)          K(I)
     OXYGEN           0.27373E-01   0.57046E-04   0.92615       16235.
     NITROGEN         0.90944E-04   0.21804E-07   0.30826E-02
0.14138E+06
     AMMONIA          0.29921E-04   0.29273E-04   0.51264E-04    1.7512
     WATER            0.78787       0.81093       0.29047E-01   0.35819E-
01
     CARBO-01         0.10913E-02   0.42278E-04   0.35608E-01    842.24
     NIACINAM         0.17827       0.18369       0.34864E-06   0.18980E-
05
     METDIAMI         0.20141E-06   0.19916E-06   0.27524E-06    1.3820
     METHYLPI         0.18373E-02   0.17647E-02   0.42264E-02    2.3950
     3-MET-01         0.16370E-02   0.16373E-02   0.16280E-02   0.99434
     NICOT-01         0.18007E-02   0.18493E-02   0.20296E-03   0.10975

BLOCK:  SP-201   MODEL: FSPLIT
------------------------------
  INLET STREAM:         S-118
  OUTLET STREAMS:       S-202       S-201
  PROPERTY OPTION SET:  RK-SOAVE  STANDARD RKS EQUATION OF STATE

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

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 83
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  SP-201   MODEL: FSPLIT (CONTINUED)
   TOTAL BALANCE
      MOLE(LBMOL/HR)           94.8327         94.8327          0.00000
      MASS(LB/HR   )           1681.80         1681.80         0.135196E-15
      ENTHALPY(BTU/HR  )     -0.890837E+07   -0.890837E+07   -0.209089E-15

                     ***  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  ***

 FRACTION OF FLOW               STRM=S-202     FRAC=          0.98900

                          ***  RESULTS  ***

 STREAM= S-202         SPLIT=          0.98900     KEY=  0    STREAM-ORDER=
1
        S-201                          0.011000          0
2

BLOCK:  SP-301   MODEL: FSPLIT
------------------------------
  INLET STREAM:         S-317
  OUTLET STREAMS:       S-319       S-318
  PROPERTY OPTION SET:  RK-SOAVE  STANDARD RKS EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1230.61         1230.61          0.00000
      MASS(LB/HR   )           22166.6         22166.6        -0.164120E-15
      ENTHALPY(BTU/HR  )     -0.153794E+09   -0.153794E+09   -0.148026E-08

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.212006E-01   LB/HR
   PRODUCT STREAMS CO2E        0.212006E-01   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  ***

 PRESSURE DROP   PSI                                     10.0000

 FRACTION OF FLOW               STRM=S-319     FRAC=          0.100000
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 84
                             NIACIN PRODUCTION
                             U-O-S BLOCK SECTION

BLOCK:  SP-301   MODEL: FSPLIT (CONTINUED)

                       ***  RESULTS  ***

 STREAM= S-319         SPLIT=          0.100000    KEY=  0    STREAM-ORDER=
1
        S-318                          0.90000           0
2

BLOCK:  SP-302   MODEL: FSPLIT
------------------------------
  INLET STREAM:          S-313
  OUTLET STREAMS:        S-315       S-314
  PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            11.1805         11.1805        0.00000
      MASS(LB/HR   )            314.592         314.592        0.180689E-15
      ENTHALPY(BTU/HR  )       -18108.1        -18108.1        0.968382E-09

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             3.44686      LB/HR
   PRODUCT STREAMS CO2E          3.44686      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  ***

 PRESSURE DROP   PSI                                 10.0000

 FRACTION OF FLOW              STRM=S-314    FRAC=       0.100000

                       ***  RESULTS  ***

 STREAM= S-315         SPLIT=          0.90000     KEY=  0    STREAM-ORDER=
2
        S-314                          0.100000          0
1
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                    03/27/2013  PAGE 85
                              NIACIN PRODUCTION
                                 STREAM SECTION

 SUBSTREAM ATTR PSD TYPE: PSD
 ----------------------------

 INTERVAL     LOWER LIMIT           UPPER LIMIT
     1          0.0        FT       6.5617-05  FT
     2        6.5617-05   FT        1.3123-04  FT
     3        1.3123-04   FT        1.9685-04  FT
     4        1.9685-04   FT        2.6247-04  FT
     5        2.6247-04   FT        3.2808-04  FT
     6        3.2808-04   FT        3.9370-04  FT
     7        3.9370-04   FT        4.5932-04  FT
     8        4.5932-04   FT        5.2493-04  FT
     9        5.2493-04   FT        5.9055-04  FT
    10        5.9055-04   FT        6.5617-04  FT
```

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 86
NIACIN PRODUCTION
STREAM SECTION

S-101 S-102 S-103 S-104 S-105

STREAM ID	S-101	S-102	S-103	S-104	S-105
FROM :	----	P-101	M-101	HX-101	C-101
TO :	P-101	M-101	HX-101	C-101	R-101
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	3306.9340	3306.9340	3340.3368	3340.3368	3340.3368
BTU/HR	-2.0341+06	-2.0332+06	-2.0469+06	-5.7939+05	-5.2259+05
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	0.0	0.0	1.1731-19	1.1731-19	1.1731-19
WATER	0.0	0.0	0.0	0.0	0.0
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	28.4590	28.4590	28.7464	28.7464	28.7464
METHYLPI	0.0	0.0	3.1607-05	3.1607-05	3.1607-05
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	0.0	0.0	4.0808-21	4.0808-21	4.0808-21
WATER	0.0	0.0	0.0	0.0	0.0
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	1.0000	1.0000	1.0000	1.0000	1.0000
METHYLPI	0.0	0.0	1.0995-06	1.0995-06	1.0995-06
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	0.0	0.0	1.9978-18	1.9978-18	1.9978-18
WATER	0.0	0.0	0.0	0.0	0.0
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	3306.9340	3306.9340	3340.3337	3340.3337	3340.3337
METHYLPI	0.0	0.0	3.1344-03	3.1344-03	3.1344-03
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 87
NIACIN PRODUCTION
STREAM SECTION

S-101 S-102 S-103 S-104 S-105 (CONTINUED)

STREAM ID	S-101	S-102	S-103	S-104	S-105
AMMONIA	0.0	0.0	5.9810-22	5.9810-22	5.9810-22
WATER	0.0	0.0	0.0	0.0	0.0
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	1.0000	1.0000	1.0000	1.0000	1.0000
METHYLPI	0.0	0.0	9.3836-07	9.3836-07	9.3836-07
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	28.4590	28.4590	28.7464	28.7464	28.7464
LB/HR	3306.9340	3306.9340	3340.3368	3340.3368	3340.3368
CUFT/HR	53.9515	53.9621	54.6159	8642.4869	3915.2157
STATE VARIABLES:					
TEMP F	77.0000	77.3730	81.1415	527.0000	560.2087
PRES PSIA	14.5038	43.5113	43.5113	33.5113	72.5189
VFRAC	0.0	0.0	0.0	1.0000	1.0000
LFRAC	1.0000	1.0000	1.0000	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-7.1476+04	-7.1442+04	-7.1207+04	-2.0155+04	-1.8179+04
BTU/LB	-615.1156	-614.8194	-612.7958	-173.4516	-156.4484
BTU/HR	-2.0341+06	-2.0332+06	-2.0469+06	-5.7939+05	-5.2259+05
ENTROPY:					
BTU/LBMOL-R	-222.0035	-221.9648	-221.5284	-157.4434	-156.8990
BTU/LB-R	-1.9105	-1.9102	-1.9064	-1.3549	-1.3502
DENSITY:					
LBMOL/CUFT	0.5275	0.5274	0.5263	3.3262-03	7.3422-03
LB/CUFT	61.2946	61.2825	61.1605	0.3865	0.8532
AVG MW	116.2000	116.2000	116.2000	116.2000	116.2000

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 88
NIACIN PRODUCTION
STREAM SECTION

S-106 S-107 S-108 S-109 S-110

STREAM ID	S-106	S-107	S-108	S-109	S-110
FROM :	R-101	D-101	D-101	P-102	C-102
TO :	D-101	C-102	P-102	M-101	HX-102
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
MAX CONV. ERROR:	0.0	0.0	-9.1223-06	0.0	0.0
TOTAL STREAM:					
LB/HR	3340.3528	3306.9499	33.4028	33.4028	3306.9499
BTU/HR	-9.7465+05	-1.5017+06	-1.3787+04	-1.3777+04	-1.3141+06
SUBSTREAM: MIXED					
PHASE:	VAPOR	VAPOR	MIXED	LIQUID	VAPOR
COMPONENTS: LBMOL/HR					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	28.4590	28.4590	1.1731-19	1.1731-19	28.4590
WATER	0.0	0.0	0.0	0.0	0.0
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.2875	3.1198-05	0.2874	0.2874	3.1198-05
METHYLPI	28.4590	28.4590	3.1607-05	3.1607-05	28.4590
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	0.4975	0.5000	4.0808-19	4.0808-19	0.5000
WATER	0.0	0.0	0.0	0.0	0.0
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	5.0251-03	5.4812-07	0.9999	0.9999	5.4812-07
METHYLPI	0.4975	0.5000	1.0995-04	1.0995-04	0.5000
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	484.6719	484.6719	1.9978-18	1.9978-18	484.6719
WATER	0.0	0.0	0.0	0.0	0.0
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	33.4033	3.6252-03	33.3997	33.3997	3.6252-03
METHYLPI	2822.2775	2822.2744	3.1344-03	3.1344-03	2822.2744
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	0.0	0.0	0.0	0.0	0.0

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 89
NIACIN PRODUCTION
STREAM SECTION

S-106 S-107 S-108 S-109 S-110 (CONTINUED)

STREAM ID	S-106	S-107	S-108	S-109	S-110
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	0.1451	0.1466	5.9811-20	5.9811-20	0.1466
WATER	0.0	0.0	0.0	0.0	0.0
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	9.9999-03	1.0962-06	0.9999	0.9999	1.0962-06
METHYLPI	0.8449	0.8534	9.3838-05	9.3838-05	0.8534
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	57.2054	56.9179	0.2875	0.2875	56.9179
LB/HR	3340.3528	3306.9499	33.4028	33.4028	3306.9499
CUFT/HR	8706.5292	2.9720+04	0.6761	0.6763	6847.9515
STATE VARIABLES:					
TEMP F	581.0000	266.2846	402.3192	402.6851	393.1779
PRES PSIA	71.6486	14.6959	20.5459	43.5113	72.5189
VFRAC	1.0000	1.0000	1.2289-08	0.0	1.0000
LFRAC	0.0	0.0	1.0000	1.0000	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.7038+04	-2.6384+04	-4.7961+04	-4.7927+04	-2.3088+04
BTU/LB	-291.7791	-454.1038	-412.7500	-412.4590	-397.3751
BTU/HR	-9.7465+05	-1.5017+06	-1.3787+04	-1.3777+04	-1.3141+06
ENTROPY:					
BTU/LBMOL-R	-79.2776	-86.4713	-188.1311	-188.1068	-85.3726
BTU/LB-R	-1.3577	-1.4883	-1.6191	-1.6188	-1.4694
DENSITY:					
LBMOL/CUFT	6.5704-03	1.9151-03	0.4252	0.4251	8.3117-03
LB/CUFT	0.3837	0.1113	49.4057	49.3902	0.4829
AVG MW	58.3923	58.1003	116.1981	116.1981	58.1003

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                      03/27/2013  PAGE 90
                             NIACIN PRODUCTION
                                STREAM SECTION

S-111 S-112 S-113 S-114 S-115
-----------------------------

STREAM ID                 S-111      S-112      S-113      S-114      S-115
FROM :                    HX-102     R-102      A-101      C-103      A-102
TO   :                    R-102      A-101      C-103      A-102      ----
CLASS:                    MIXCIPSD   MIXCIPSD   MIXCIPSD   MIXCIPSD   MIXCIPSD
TOTAL STREAM:
  LB/HR                  3306.9499  3307.1178   656.4753   656.4753   174.6730
  BTU/HR                -1.0212+06  1.5815+06 -6.1968+05 -3.6190+05 -1.1704+05
SUBSTREAM: MIXED
PHASE:                    VAPOR      VAPOR      VAPOR      VAPOR      VAPOR
COMPONENTS: LBMOL/HR
  OXYGEN                   0.0        0.0        0.0        0.0        0.0
  HYDROGEN                 0.0       84.5231    84.5231    84.5231    84.5231
  NITROGEN                 0.0        0.0        0.0        0.0        0.0
  AMMONIA                 28.4590    28.4590    28.4590    28.4590     0.2516
  WATER                    0.0        0.0        0.0        0.0     4.9598-11
  CARBO-01                 0.0        0.0        0.0        0.0        0.0
  NIACINAM                 0.0        0.0        0.0        0.0        0.0
  METDIAMI               3.1198-05  3.1198-05  3.1756-19  3.1756-19    0.0
  METHYLPI                28.4590     0.2846   1.4805-06  1.4805-06  3.1187-08
  3-MET-01                 0.0       28.1744   1.5192-02  1.5192-02  7.5508-08
  NICOT-01                 0.0        0.0        0.0        0.0        0.0
  AMMONICO                 0.0        0.0        0.0        0.0        0.0
COMPONENTS: MOLE FRAC
  OXYGEN                   0.0        0.0        0.0        0.0        0.0
  HYDROGEN                 0.0        0.5976     0.7480     0.7480     0.9970
  NITROGEN                 0.0        0.0        0.0        0.0        0.0
  AMMONIA                  0.5000     0.2012     0.2519     0.2519   2.9677-03
  WATER                    0.0        0.0        0.0        0.0     5.8506-13
  CARBO-01                 0.0        0.0        0.0        0.0        0.0
  NIACINAM                 0.0        0.0        0.0        0.0        0.0
  METDIAMI               5.4812-07  2.2057-07  2.8103-21  2.8103-21    0.0
  METHYLPI                 0.5000   2.0121-03  1.3103-08  1.3103-08  3.6788-10
  3-MET-01                 0.0        0.1992   1.3445-04  1.3445-04  8.9070-10
  NICOT-01                 0.0        0.0        0.0        0.0        0.0
  AMMONICO                 0.0        0.0        0.0        0.0        0.0
COMPONENTS: LB/HR
  OXYGEN                   0.0        0.0        0.0        0.0        0.0
  HYDROGEN                 0.0      170.3884   170.3884   170.3884   170.3884
  NITROGEN                 0.0        0.0        0.0        0.0        0.0
  AMMONIA                484.6719   484.6719   484.6719   484.6719     4.2846
  WATER                    0.0        0.0        0.0        0.0     8.9352-10
  CARBO-01                 0.0        0.0        0.0        0.0        0.0
  NIACINAM                 0.0        0.0        0.0        0.0        0.0
  METDIAMI               3.6252-03  3.6252-03  3.6900-17  3.6900-17    0.0
  METHYLPI              2822.2744    28.2227   1.4683-04  1.4683-04  3.0928-06
  3-MET-01                 0.0     2623.8311     1.4148     1.4148   7.0320-06
  NICOT-01                 0.0        0.0        0.0        0.0        0.0
  AMMONICO                 0.0        0.0        0.0        0.0        0.0
COMPONENTS: MASS FRAC
  OXYGEN                   0.0        0.0        0.0        0.0        0.0
  HYDROGEN                 0.0      5.1522-02    0.2596     0.2596     0.9755
  NITROGEN                 0.0        0.0        0.0        0.0        0.0
```

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                      03/27/2013  PAGE 91
                             NIACIN PRODUCTION
                                STREAM SECTION

S-111 S-112 S-113 S-114 S-115 (CONTINUED)

STREAM ID                 S-111      S-112      S-113      S-114      S-115

  AMMONIA                  0.1466     0.1466     0.7383     0.7383   2.4529-02
  WATER                    0.0        0.0        0.0        0.0     5.1154-12
  CARBO-01                 0.0        0.0        0.0        0.0        0.0
  NIACINAM                 0.0        0.0        0.0        0.0        0.0
  METDIAMI               1.0962-06  1.0962-06  5.6209-20  5.6209-20    0.0
  METHYLPI                 0.8534   8.5339-03  2.2366-07  2.2366-07  1.7706-08
  3-MET-01                 0.0        0.7934   2.1552-03  2.1552-03  4.0258-08
  NICOT-01                 0.0        0.0        0.0        0.0        0.0
  AMMONICO                 0.0        0.0        0.0        0.0        0.0
TOTAL FLOW:
  LBMOL/HR                56.9179   141.4410   112.9972   112.9972    84.7747
  LB/HR                 3306.9499  3307.1178   656.4753   656.4753   174.6730
  CUFT/HR               9682.3015  3.6436+04  1.4104+04  5536.6433  1844.5556
STATE VARIABLES:
  TEMP   F               554.0000   554.0000     5.9902   313.6720  -117.8784
  PRES   PSIA             62.5189    42.2136    40.0000   170.0000   170.0000
  VFRAC                    1.0000     1.0000     1.0000     1.0000     1.0000
  LFRAC                    0.0        0.0        0.0        0.0        0.0
  SFRAC                    0.0        0.0        0.0        0.0        0.0
ENTHALPY:
  BTU/LBMOL            -1.7941+04  1.1181+04 -5483.9974 -3202.7557 -1380.6474
  BTU/LB                -308.7899   478.2133  -943.9450  -551.2813  -670.0745
  BTU/HR               -1.0212+06  1.5815+06 -6.1968+05 -3.6190+05 -1.1704+05
ENTROPY:
  BTU/LBMOL-R             -79.5689    -9.6793    -7.8642    -6.9901    -7.9663
  BTU/LB-R                 -1.3695    -0.4140    -1.3536    -1.2032    -3.8663
DENSITY:
  LBMOL/CUFT             5.8786-03  3.8819-03  8.0117-03  2.0409-02  4.5959-02
  LB/CUFT                  0.3415   9.0765-02  4.6545-02    0.1186   9.4697-02
AVG MW                    58.1003    23.3816     5.8097     5.8097     2.0604
```

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 92
NIACIN PRODUCTION
STREAM SECTION

S-116 S-117 S-118 S-119 S-201

STREAM ID	S-116	S-117	S-118	S-119	S-201
FROM :	----	P-103	A-102	A-101	SP-201
TO :	P-103	A-102	SP-201	M-201	M-301
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	1200.0000	1200.0000	1681.8023	2650.6425	18.4998
BTU/HR	-8.2594+06	-8.2575+06	-8.9084+06	1.0781+06	-9.7992+04
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	MIXED	MIXED	MIXED
COMPONENTS: LBMOL/HR					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	1.5060-14	7.6711-14	1.6566-16
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	0.0	0.0	28.2074	1.0772-07	0.3103
WATER	66.6101	66.6101	66.6101	0.0	0.7327
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	0.0	0.0	3.1198-05	0.0
METHYLPI	0.0	0.0	1.4494-06	0.2846	1.5943-08
3-MET-01	0.0	0.0	1.5192-02	28.1592	1.6711-04
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	1.5880-16	2.6969-15	1.5880-16
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	0.0	0.0	0.2974	3.7871-09	0.2974
WATER	1.0000	1.0000	0.7024	0.0	0.7024
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	0.0	0.0	1.0968-06	0.0
METHYLPI	0.0	0.0	1.5283-08	1.0005-02	1.5283-08
3-MET-01	0.0	0.0	1.6020-04	0.9900	1.6020-04
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	3.0358-14	1.5464-13	3.3394-16
NITROGEN	0.0	0.0	0.0	0.0	0.0
AMMONIA	0.0	0.0	480.3873	1.8345-06	5.2843
WATER	1200.0000	1200.0000	1200.0000	0.0	13.2000
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	0.0	0.0	3.6252-03	0.0
METHYLPI	0.0	0.0	1.4373-04	28.2226	1.5811-06
3-MET-01	0.0	0.0	1.4148	2622.4163	1.5563-02
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	0.0	0.0	0.0	0.0	0.0
HYDROGEN	0.0	0.0	1.8051-17	5.8341-17	1.8051-17
NITROGEN	0.0	0.0	0.0	0.0	0.0

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 93
NIACIN PRODUCTION
STREAM SECTION

S-116 S-117 S-118 S-119 S-201 (CONTINUED)

STREAM ID	S-116	S-117	S-118	S-119	S-201
AMMONIA	0.0	0.0	0.2856	6.9211-10	0.2856
WATER	1.0000	1.0000	0.7135	0.0	0.7135
CARBO-01	0.0	0.0	0.0	0.0	0.0
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	0.0	0.0	1.3677-06	0.0
METHYLPI	0.0	0.0	8.5464-08	1.0647-02	8.5464-08
3-MET-01	0.0	0.0	8.4125-04	0.9894	8.4125-04
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	66.6101	66.6101	94.8327	28.4438	1.0432
LB/HR	1200.0000	1200.0000	1681.8023	2650.6425	18.4998
CUFT/HR	19.4761	19.4862	35.1089	53.5694	0.3862
STATE VARIABLES:					
TEMP F	90.0000	90.9526	224.7170	366.2599	224.7170
PRES PSIA	15.0000	170.0000	170.0000	40.0000	170.0000
VFRAC	0.0	0.0	5.1152-06	4.4361-07	5.1152-06
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.2400+05	-1.2397+05	-9.3938+04	3.7904+04	-9.3938+04
BTU/LB	-6882.7988	-6881.2243	-5296.9162	406.7394	-5296.9162
BTU/HR	-8.2594+06	-8.2575+06	-8.9084+06	1.0781+06	-9.7992+04
ENTROPY:					
BTU/LBMOL-R	-40.3951	-40.3635	-37.1520	-71.4089	-37.1520
BTU/LB-R	-2.2423	-2.2405	-2.0949	-0.7663	-2.0949
DENSITY:					
LBMOL/CUFT	3.4201	3.4183	2.7011	0.5310	2.7011
LB/CUFT	61.6141	61.5820	47.9024	49.4806	47.9024
AVG MW	18.0153	18.0153	17.7344	93.1888	17.7344

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 94
NIACIN PRODUCTION
STREAM SECTION

S-202 S-203 S-203A S-204 S-205

STREAM ID	S-202	S-203	S-203A	S-204	S-205
FROM :	SP-201	HX-201	M-201	----	R-201
TO :	M-201	R-201	HX-201	R-201	HX-202A
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	1663.3024	4313.9450	4313.9450	1481.4509	5795.3959
BTU/HR	-8.8104+06	-5.1319+06	-7.7323+06	-444.5190	-1.1013+07
SUBSTREAM: MIXED					
PHASE:	MIXED	VAPOR	MIXED	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
OXYGEN	0.0	0.0	0.0	46.2971	4.2400
HYDROGEN	1.4894-14	9.1605-14	9.1605-14	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	1.4087-02
AMMONIA	27.8971	27.8971	27.8971	0.0	4.6348-03
WATER	65.8774	65.8774	65.8774	0.0	149.6534
CARBO-01	0.0	0.0	0.0	0.0	0.1690
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	3.1198-05	3.1198-05	0.0	3.1198-05
METHYLPI	1.4334-06	0.2846	0.2846	0.0	0.2846
3-MET-01	1.5025-02	28.1742	28.1742	0.0	0.2536
NICOT-01	0.0	0.0	0.0	0.0	27.8925
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	0.0	0.0	0.0	1.0000	2.3232-02
HYDROGEN	1.5880-16	7.4943-16	7.4943-16	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	7.7185-05
AMMONIA	0.2974	0.2282	0.2282	0.0	2.5394-05
WATER	0.7024	0.5389	0.5389	0.0	0.8200
CARBO-01	0.0	0.0	0.0	0.0	9.2621-04
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	2.5523-07	2.5523-07	0.0	1.7093-07
METHYLPI	1.5283-08	2.3282-03	2.3282-03	0.0	1.5593-03
3-MET-01	1.6020-04	0.2305	0.2305	0.0	1.3893-03
NICOT-01	0.0	0.0	0.0	0.0	0.1528
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	0.0	0.0	0.0	1481.4509	135.6763
HYDROGEN	3.0024-14	1.8466-13	1.8466-13	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.3946
AMMONIA	475.1030	475.1031	475.1031	0.0	7.8933-02
WATER	1186.8000	1186.8000	1186.8000	0.0	2696.0476
CARBO-01	0.0	0.0	0.0	0.0	7.4396
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	3.6252-03	3.6252-03	0.0	3.6252-03
METHYLPI	1.4215-04	28.2227	28.2227	0.0	28.2227
3-MET-01	1.3993	2623.8156	2623.8156	0.0	23.6143
NICOT-01	0.0	0.0	0.0	0.0	2903.9180
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	0.0	0.0	0.0	1.0000	2.3411-02
HYDROGEN	1.8051-17	4.2806-17	4.2806-17	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	6.8093-05

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 95
NIACIN PRODUCTION
STREAM SECTION

S-202 S-203 S-203A S-204 S-205 (CONTINUED)

STREAM ID	S-202	S-203	S-203A	S-204	S-205
AMMONIA	0.2856	0.1101	0.1101	0.0	1.3620-05
WATER	0.7135	0.2751	0.2751	0.0	0.4652
CARBO-01	0.0	0.0	0.0	0.0	1.2837-03
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	8.4034-07	8.4034-07	0.0	6.2553-07
METHYLPI	8.5464-08	6.5422-03	6.5422-03	0.0	4.8699-03
3-MET-01	8.4125-04	0.6082	0.6082	0.0	4.0747-03
NICOT-01	0.0	0.0	0.0	0.0	0.5011
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	93.7895	122.2333	122.2333	46.2971	182.5118
LB/HR	1663.3024	4313.9450	4313.9450	1481.4509	5795.3959
CUFT/HR	34.7227	4.7201+04	1287.3168	6748.4266	7.2571+04
STATE VARIABLES:					
TEMP F	224.7170	626.0000	158.8554	77.0000	626.0000
PRES PSIA	170.0000	30.0000	40.0000	39.4503	29.1298
VFRAC	5.1152-06	1.0000	6.0995-02	1.0000	1.0000
LFRAC	1.0000	0.0	0.9390	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-9.3938+04	-4.1985+04	-6.3258+04	-9.6014	-6.0343+04
BTU/LB	-5296.9162	-1189.6179	-1792.3860	-0.3001	-1900.3591
BTU/HR	-8.8104+06	-5.1319+06	-7.7323+06	-444.5190	-1.1013+07
ENTROPY:					
BTU/LBMOL-R	-37.1520	-15.0794	-45.0383	-1.9758	-3.7817
BTU/LB-R	-2.0949	-0.4273	-1.2761	-6.1746-02	-0.1191
DENSITY:					
LBMOL/CUFT	2.7011	2.5896-03	9.4952-02	6.8604-03	2.5149-03
LB/CUFT	47.9024	9.1395-02	3.3511	0.2195	7.9858-02
AVG MW	17.7344	35.2927	35.2927	31.9988	31.7535

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 96
NIACIN PRODUCTION
STREAM SECTION

S-206 S-206A S-207 S-208 S-209

STREAM ID	S-206	S-206A	S-207	S-208	S-209
FROM :	HX-202B	HX-202A	R-202A	SEP-201	B-201
TO :	R-202A	HX-202B	SEP-201	B-201	M-202
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	5795.3959	5795.3959	5795.2158	148.4361	148.4361
BTU/HR	-1.5485+07	-1.5390+07	-1.6613+07	-4.2756+04	-3.6942+04
SUBSTREAM: MIXED					
PHASE:	MIXED	MIXED	MIXED	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
OXYGEN	4.2400	4.2400	4.2400	4.2320	4.2320
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	1.4087-02	1.4087-02	1.4087-02	1.4084-02	1.4084-02
AMMONIA	4.6348-03	4.6348-03	4.6348-03	2.4981-04	2.4981-04
WATER	149.6534	149.6534	122.0399	0.1420	0.1420
CARBO-01	0.1690	0.1690	0.1690	0.1631	0.1631
NIACINAM	0.0	0.0	27.6135	1.7024-06	1.7024-06
METDIAMI	3.1198-05	3.1198-05	3.1198-05	1.3407-06	1.3407-06
METHYLPI	0.2846	0.2846	0.2846	2.0554-02	2.0554-02
3-MET-01	0.2536	0.2536	0.2536	7.9390-03	7.9390-03
NICOT-01	27.8925	27.8925	0.2789	9.9121-04	9.9121-04
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	2.3232-02	2.3232-02	2.7373-02	0.9238	0.9238
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	7.7185-05	7.7185-05	9.0944-05	3.0745-03	3.0745-03
AMMONIA	2.5394-05	2.5394-05	2.9921-05	5.4533-05	5.4533-05
WATER	0.8200	0.8200	0.7879	3.1000-02	3.1000-02
CARBO-01	9.2621-04	9.2621-04	1.0913-03	3.5602-02	3.5602-02
NIACINAM	0.0	0.0	0.1783	3.7163-07	3.7163-07
METDIAMI	1.7093-07	1.7093-07	2.0141-07	2.9267-07	2.9267-07
METHYLPI	1.5593-03	1.5593-03	1.8373-03	4.4868-03	4.4868-03
3-MET-01	1.3893-03	1.3893-03	1.6370-03	1.7330-03	1.7330-03
NICOT-01	0.1528	0.1528	1.8007-03	2.1638-04	2.1638-04
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	135.6763	135.6763	135.6763	135.4200	135.4200
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.3946	0.3946	0.3946	0.3945	0.3945
AMMONIA	7.8933-02	7.8933-02	7.8933-02	4.2545-03	4.2545-03
WATER	2696.0476	2696.0476	2198.5821	2.5583	2.5583
CARBO-01	7.4396	7.4396	7.4396	7.1777	7.1777
NIACINAM	0.0	0.0	3372.1643	2.0790-04	2.0790-04
METDIAMI	3.6252-03	3.6252-03	3.6252-03	1.5579-04	1.5579-04
METHYLPI	28.2227	28.2227	28.2227	2.0383	2.0383
3-MET-01	23.6143	23.6143	23.6143	0.7393	0.7393
NICOT-01	2903.9180	2903.9180	29.0392	0.1032	0.1032
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	2.3411-02	2.3411-02	2.3412-02	0.9123	0.9123
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	6.8093-05	6.8093-05	6.8096-05	2.6580-03	2.6580-03

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 97
NIACIN PRODUCTION
STREAM SECTION

S-206 S-206A S-207 S-208 S-209 (CONTINUED)

STREAM ID	S-206	S-206A	S-207	S-208	S-209
AMMONIA	1.3620-05	1.3620-05	1.3620-05	2.8662-05	2.8662-05
WATER	0.4652	0.4652	0.3794	1.7235-02	1.7235-02
CARBO-01	1.2837-03	1.2837-03	1.2838-03	4.8356-02	4.8356-02
NIACINAM	0.0	0.0	0.5819	1.4006-06	1.4006-06
METDIAMI	6.2553-07	6.2553-07	6.2554-07	1.0495-06	1.0495-06
METHYLPI	4.8699-03	4.8699-03	4.8700-03	1.3732-02	1.3732-02
3-MET-01	4.0747-03	4.0747-03	4.0748-03	4.9809-03	4.9809-03
NICOT-01	0.5011	0.5011	5.0109-03	6.9522-04	6.9522-04
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	182.5118	182.5118	154.8983	4.5810	4.5810
LB/HR	5795.3959	5795.3959	5795.2158	148.4361	148.4361
CUFT/HR	1457.4053	1245.1048	1865.6338	1789.2957	1094.1083
STATE VARIABLES:					
TEMP F	77.0000	100.0000	77.0000	77.0000	249.4160
PRES PSIA	19.1298	24.1298	14.7298	14.7298	31.8503
VFRAC	2.4904-02	2.5426-02	2.9574-02	1.0000	1.0000
LFRAC	0.9751	0.9746	0.9704	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-8.4846+04	-8.4324+04	-1.0725+05	-9333.3538	-8064.2282
BTU/LB	-2672.0078	-2655.5837	-2866.6394	-288.0411	-248.8740
BTU/HR	-1.5485+07	-1.5390+07	-1.6613+07	-4.2756+04	-3.6942+04
ENTROPY:					
BTU/LBMOL-R	-38.1308	-37.1920	-52.1945	-0.4678	5.0892-02
BTU/LB-R	-1.2008	-1.1713	-1.3951	-1.4437-02	1.5706-03
DENSITY:					
LBMOL/CUFT	0.1252	0.1466	8.3027-02	2.5602-03	4.1869-03
LB/CUFT	3.9765	4.6545	3.1063	8.2958-02	0.1357
AVG MW	31.7535	31.7535	37.4130	32.4028	32.4028

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 98
NIACIN PRODUCTION
STREAM SECTION

S-210 S-211 S-212 S-213 S-214

STREAM ID	S-210	S-211	S-212	S-213	S-214
FROM :	SEP-201	P-201	M-202	HX-203	R-202B
TO :	P-201	M-202	HX-203	R-202B	SEP-202
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	5646.7798	5646.7798	5795.2158	5795.2158	5795.2158
BTU/HR	-1.6570+07	-1.6569+07	-1.6606+07	-1.6613+07	-1.6613+07
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	MIXED	MIXED	MIXED
COMPONENTS: LBMOL/HR					
OXYGEN	8.0101-03	8.0101-03	4.2400	4.2400	4.2400
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	3.0611-06	3.0611-06	1.4087-02	1.4087-02	1.4087-02
AMMONIA	4.3849-03	4.3849-03	4.6348-03	4.6348-03	4.6348-03
WATER	121.8978	121.8978	122.0399	122.0399	122.0399
CARBO-01	5.9518-03	5.9518-03	0.1690	0.1690	0.1690
NIACINAM	27.6135	27.6135	27.6135	27.6135	27.6135
METDIAMI	2.9857-05	2.9857-05	3.1198-05	3.1198-05	3.1198-05
METHYLPI	0.2640	0.2640	0.2846	0.2846	0.2846
3-MET-01	0.2456	0.2456	0.2536	0.2536	0.2536
NICOT-01	0.2779	0.2779	0.2789	0.2789	0.2789
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	5.3288-05	5.3288-05	2.7373-02	2.7373-02	2.7373-02
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	2.0364-08	2.0364-08	9.0944-05	9.0944-05	9.0944-05
AMMONIA	2.9171-05	2.9171-05	2.9921-05	2.9921-05	2.9921-05
WATER	0.8109	0.8109	0.7879	0.7879	0.7879
CARBO-01	3.9595-05	3.9595-05	1.0913-03	1.0913-03	1.0913-03
NIACINAM	0.1837	0.1837	0.1783	0.1783	0.1783
METDIAMI	1.9863-07	1.9863-07	2.0141-07	2.0141-07	2.0141-07
METHYLPI	1.7565-03	1.7565-03	1.8373-03	1.8373-03	1.8373-03
3-MET-01	1.6341-03	1.6341-03	1.6370-03	1.6370-03	1.6370-03
NICOT-01	1.8490-03	1.8490-03	1.8007-03	1.8007-03	1.8007-03
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	0.2563	0.2563	135.6763	135.6763	135.6763
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	8.5752-05	8.5752-05	0.3946	0.3946	0.3946
AMMONIA	7.4678-02	7.4678-02	7.8933-02	7.8933-02	7.8933-02
WATER	2196.0238	2196.0238	2198.5821	2198.5821	2198.5821
CARBO-01	0.2619	0.2619	7.4396	7.4396	7.4396
NIACINAM	3372.1641	3372.1641	3372.1643	3372.1643	3372.1643
METDIAMI	3.4694-03	3.4694-03	3.6252-03	3.6252-03	3.6252-03
METHYLPI	26.1844	26.1844	28.2227	28.2227	28.2227
3-MET-01	22.8750	22.8750	23.6143	23.6143	23.6143
NICOT-01	28.9360	28.9360	29.0392	29.0392	29.0392
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	4.5391-05	4.5391-05	2.3412-02	2.3412-02	2.3412-02
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	1.5186-08	1.5186-08	6.8096-05	6.8096-05	6.8096-05

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 99
NIACIN PRODUCTION
STREAM SECTION

S-210 S-211 S-212 S-213 S-214 (CONTINUED)

STREAM ID	S-210	S-211	S-212	S-213	S-214
AMMONIA	1.3225-05	1.3225-05	1.3620-05	1.3620-05	1.3620-05
WATER	0.3889	0.3889	0.3794	0.3794	0.3794
CARBO-01	4.6387-05	4.6387-05	1.2838-03	1.2838-03	1.2838-03
NIACINAM	0.5972	0.5972	0.5819	0.5819	0.5819
METDIAMI	6.1440-07	6.1440-07	6.2554-07	6.2554-07	6.2554-07
METHYLPI	4.6371-03	4.6371-03	4.8700-03	4.8700-03	4.8700-03
3-MET-01	4.0510-03	4.0510-03	4.0748-03	4.0748-03	4.0748-03
NICOT-01	5.1243-03	5.1243-03	5.0109-03	5.0109-03	5.0109-03
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	150.3174	150.3174	154.8983	154.8983	154.8983
LB/HR	5646.7798	5646.7798	5795.2158	5795.2158	5795.2158
CUFT/HR	76.3381	76.3426	946.9293	1397.6407	1804.4997
STATE VARIABLES:					
TEMP F	77.0000	77.1252	78.9689	77.0000	77.0000
PRES PSIA	14.7298	29.7298	29.7298	19.7298	15.2298
VFRAC	0.0	0.0	2.8952-02	2.9258-02	2.9534-02
LFRAC	1.0000	1.0000	0.9710	0.9707	0.9705
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.1023+05	-1.1023+05	-1.0721+05	-1.0725+05	-1.0725+05
BTU/LB	-2934.4226	-2934.2957	-2865.5125	-2866.7578	-2866.6553
BTU/HR	-1.6570+07	-1.6569+07	-1.6606+07	-1.6613+07	-1.6613+07
ENTROPY:					
BTU/LBMOL-R	-53.7709	-53.7656	-52.1603	-52.2210	-52.1977
BTU/LB-R	-1.4314	-1.4312	-1.3942	-1.3958	-1.3952
DENSITY:					
LBMOL/CUFT	1.9691	1.9690	0.1636	0.1108	8.5840-02
LB/CUFT	73.9706	73.9663	6.1200	4.1464	3.2115
AVG MW	37.5657	37.5657	37.4130	37.4130	37.4130

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 100
NIACIN PRODUCTION
STREAM SECTION

S-215 S-216 S-217 S-218 S-219

STREAM ID	S-215	S-216	S-217	S-218	S-219
FROM :	SEP-202	B-202	SEP-202	P-202	M-203
TO :	B-202	M-203	P-202	M-203	HX-204
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	148.2402	148.2402	5646.9756	5646.9756	5795.2158
BTU/HR	-4.2211+04	-3.7111+04	-1.6571+07	-1.6570+07	-1.6607+07
SUBSTREAM: MIXED					
PHASE:	VAPOR	VAPOR	LIQUID	LIQUID	MIXED
COMPONENTS: LBMOL/HR					
OXYGEN	4.2318	4.2318	8.2929-03	8.2929-03	4.2400
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	1.4084-02	1.4084-02	3.1694-06	3.1694-06	1.4087-02
AMMONIA	2.4176-04	2.4176-04	4.3930-03	4.3930-03	4.6348-03
WATER	0.1372	0.1372	121.9027	121.9027	122.0399
CARBO-01	0.1629	0.1629	6.1540-03	6.1540-03	0.1690
NIACINAM	1.6458-06	1.6458-06	27.6135	27.6135	27.6135
METDIAMI	1.2978-06	1.2978-06	2.9900-05	2.9900-05	3.1198-05
METHYLPI	1.9912-02	1.9912-02	0.2647	0.2647	0.2846
3-MET-01	7.6803-03	7.6803-03	0.2459	0.2459	0.2536
NICOT-01	9.5816-04	9.5816-04	0.2780	0.2780	0.2789
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	0.9250	0.9250	5.5167-05	5.5167-05	2.7373-02
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	3.0786-03	3.0786-03	2.1084-08	2.1084-08	9.0944-05
AMMONIA	5.2848-05	5.2848-05	2.9224-05	2.9224-05	2.9921-05
WATER	2.9991-02	2.9991-02	0.8109	0.8109	0.7879
CARBO-01	3.5607-02	3.5607-02	4.0938-05	4.0938-05	1.0913-03
NIACINAM	3.5976-07	3.5976-07	0.1837	0.1837	0.1783
METDIAMI	2.8368-07	2.8368-07	1.9890-07	1.9890-07	2.0141-07
METHYLPI	4.3526-03	4.3526-03	1.7607-03	1.7607-03	1.8373-03
3-MET-01	1.6789-03	1.6789-03	1.6357-03	1.6357-03	1.6370-03
NICOT-01	2.0945-04	2.0945-04	1.8491-03	1.8491-03	1.8007-03
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	135.4110	135.4110	0.2654	0.2654	135.6763
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.3945	0.3945	8.8787-05	8.8787-05	0.3946
AMMONIA	4.1174-03	4.1174-03	7.4815-02	7.4815-02	7.8933-02
WATER	2.4717	2.4717	2196.1104	2196.1104	2198.5821
CARBO-01	7.1688	7.1688	0.2708	0.2708	7.4396
NIACINAM	2.0098-04	2.0098-04	3372.1641	3372.1641	3372.1643
METDIAMI	1.5080-04	1.5080-04	3.4744-03	3.4744-03	3.6252-03
METHYLPI	1.9747	1.9747	26.2481	26.2481	28.2227
3-MET-01	0.7153	0.7153	22.8991	22.8991	23.6143
NICOT-01	9.9755-02	9.9755-02	28.9394	28.9394	29.0392
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	0.9135	0.9135	4.6992-05	4.6992-05	2.3412-02
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	2.6615-03	2.6615-03	1.5723-08	1.5723-08	6.8096-05

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 101
NIACIN PRODUCTION
STREAM SECTION

S-215 S-216 S-217 S-218 S-219 (CONTINUED)

STREAM ID	S-215	S-216	S-217	S-218	S-219
AMMONIA	2.7775-05	2.7775-05	1.3249-05	1.3249-05	1.3620-05
WATER	1.6674-02	1.6674-02	0.3889	0.3889	0.3794
CARBO-01	4.8359-02	4.8359-02	4.7961-05	4.7961-05	1.2838-03
NIACINAM	1.3558-06	1.3558-06	0.5972	0.5972	0.5819
METDIAMI	1.0173-06	1.0173-06	6.1526-07	6.1526-07	6.2554-07
METHYLPI	1.3321-02	1.3321-02	4.6482-03	4.6482-03	4.8700-03
3-MET-01	4.8250-03	4.8250-03	4.0551-03	4.0551-03	4.0748-03
NICOT-01	6.7293-04	6.7293-04	5.1248-03	5.1248-03	5.0109-03
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	4.5747	4.5747	150.3236	150.3236	154.8983
LB/HR	148.2402	148.2402	5646.9756	5646.9756	5795.2158
CUFT/HR	1728.1584	1117.7900	76.3413	76.3458	931.7176
STATE VARIABLES:					
TEMP F	77.0000	228.9080	77.0000	77.1252	78.7705
PRES PSIA	15.2298	30.2298	15.2298	30.2298	30.2298
VFRAC	1.0000	1.0000	0.0	0.0	2.8936-02
LFRAC	0.0	0.0	1.0000	1.0000	0.9711
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-9227.0644	-8112.1827	-1.1023+05	-1.1023+05	-1.0721+05
BTU/LB	-284.7491	-250.3437	-2934.4335	-2934.3066	-2865.6515
BTU/HR	-4.2211+04	-3.7111+04	-1.6571+07	-1.6570+07	-1.6607+07
ENTROPY:					
BTU/LBMOL-R	-0.5068	-3.9100-02	-53.7708	-53.7655	-52.1710
BTU/LB-R	-1.5641-02	-1.2066-03	-1.4314	-1.4312	-1.3945
DENSITY:					
LBMOL/CUFT	2.6472-03	4.0927-03	1.9691	1.9690	0.1663
LB/CUFT	8.5779-02	0.1326	73.9701	73.9658	6.2199
AVG MW	32.4042	32.4042	37.5655	37.5655	37.4130

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 102
NIACIN PRODUCTION
STREAM SECTION

S-220 S-221 S-222 S-223 S-224

STREAM ID	S-220	S-221	S-222	S-223	S-224
FROM :	HX-204	R-202C	SEP-203	B-203	SEP-203
TO :	R-202C	SEP-203	B-203	M-204	P-203
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	5795.2158	5795.2158	148.0557	148.0557	5647.1601
BTU/HR	-1.6614+07	-1.6613+07	-4.1700+04	-3.5025+04	-1.6571+07
SUBSTREAM: MIXED					
PHASE:	MIXED	MIXED	VAPOR	VAPOR	LIQUID
COMPONENTS: LBMOL/HR					
OXYGEN	4.2400	4.2400	4.2315	4.2315	8.5757-03
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	1.4087-02	1.4087-02	1.4084-02	1.4084-02	3.2778-06
AMMONIA	4.6348-03	4.6348-03	2.3422-04	2.3422-04	4.4005-03
WATER	122.0399	122.0399	0.1327	0.1327	121.9071
CARBO-01	0.1690	0.1690	0.1627	0.1627	6.3557-03
NIACINAM	27.6135	27.6135	1.5929-06	1.5929-06	27.6135
METDIAMI	3.1198-05	3.1198-05	1.2575-06	1.2575-06	2.9940-05
METHYLPI	0.2846	0.2846	1.9310-02	1.9310-02	0.2653
3-MET-01	0.2536	0.2536	7.4381-03	7.4381-03	0.2461
NICOT-01	0.2789	0.2789	9.2729-04	9.2729-04	0.2780
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	2.7373-02	2.7373-02	0.9262	0.9262	5.7046-05
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	9.0944-05	9.0944-05	3.0826-03	3.0826-03	2.1804-08
AMMONIA	2.9921-05	2.9921-05	5.1264-05	5.1264-05	2.9273-05
WATER	0.7879	0.7879	2.9047-02	2.9047-02	0.8109
CARBO-01	1.0913-03	1.0913-03	3.5608-02	3.5608-02	4.2278-05
NIACINAM	0.1783	0.1783	3.4864-07	3.4864-07	0.1837
METDIAMI	2.0141-07	2.0141-07	2.7524-07	2.7524-07	1.9916-07
METHYLPI	1.8373-03	1.8373-03	4.2264-03	4.2264-03	1.7647-03
3-MET-01	1.6370-03	1.6370-03	1.6280-03	1.6280-03	1.6373-03
NICOT-01	1.8007-03	1.8007-03	2.0296-04	2.0296-04	1.8493-03
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	135.6763	135.6763	135.4019	135.4019	0.2744
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.3946	0.3946	0.3945	0.3945	9.1823-05
AMMONIA	7.8933-02	7.8933-02	3.9888-03	3.9888-03	7.4944-02
WATER	2198.5821	2198.5821	2.3908	2.3908	2196.1913
CARBO-01	7.4396	7.4396	7.1599	7.1599	0.2797
NIACINAM	3372.1643	3372.1643	1.9452-04	1.9452-04	3372.1641
METDIAMI	3.6252-03	3.6252-03	1.4613-04	1.4613-04	3.4790-03
METHYLPI	28.2227	28.2227	1.9150	1.9150	26.3078
3-MET-01	23.6143	23.6143	0.6927	0.6927	22.9216
NICOT-01	29.0392	29.0392	9.6541-02	9.6541-02	28.9426
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	2.3412-02	2.3412-02	0.9145	0.9145	4.8593-05
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	6.8096-05	6.8096-05	2.6648-03	2.6648-03	1.6260-08

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 103
NIACIN PRODUCTION
STREAM SECTION

S-220 S-221 S-222 S-223 S-224 (CONTINUED)

STREAM ID	S-220	S-221	S-222	S-223	S-224
AMMONIA	1.3620-05	1.3620-05	2.6941-05	2.6941-05	1.3271-05
WATER	0.3794	0.3794	1.6148-02	1.6148-02	0.3889
CARBO-01	1.2838-03	1.2838-03	4.8360-02	4.8360-02	4.9531-05
NIACINAM	0.5819	0.5819	1.3139-06	1.3139-06	0.5971
METDIAMI	6.2554-07	6.2554-07	9.8697-07	9.8697-07	6.1607-07
METHYLPI	4.8700-03	4.8700-03	1.2934-02	1.2934-02	4.6586-03
3-MET-01	4.0748-03	4.0748-03	4.6787-03	4.6787-03	4.0590-03
NICOT-01	5.0109-03	5.0109-03	6.5206-04	6.5206-04	5.1252-03
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	154.8983	154.8983	4.5689	4.5689	150.3294
LB/HR	5795.2158	5795.2158	148.0557	148.0557	5647.1601
CUFT/HR	1363.9141	1747.3886	1671.0452	954.9285	76.3443
STATE VARIABLES:					
TEMP F	77.0000	77.0000	77.0000	275.3011	77.0000
PRES PSIA	20.2298	15.7298	15.7298	37.7298	15.7298
VFRAC	2.9234-02	2.9496-02	1.0000	1.0000	0.0
LFRAC	0.9708	0.9705	0.0	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.0725+05	-1.0725+05	-9127.0909	-7665.9271	-1.1023+05
BTU/LB	-2866.7660	-2866.6700	-281.6537	-236.5635	-2934.4432
BTU/HR	-1.6614+07	-1.6613+07	-4.1700+04	-3.5025+04	-1.6571+07
ENTROPY:					
BTU/LBMOL-R	-52.2231	-52.2007	-0.5454	3.2903-02	-53.7707
BTU/LB-R	-1.3959	-1.3953	-1.6832-02	1.0153-03	-1.4314
DENSITY:					
LBMOL/CUFT	0.1136	8.8646-02	2.7341-03	4.7845-03	1.9691
LB/CUFT	4.2490	3.3165	8.8601-02	0.1550	73.9696
AVG MW	37.4130	37.4130	32.4054	32.4054	37.5652

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 104
NIACIN PRODUCTION
STREAM SECTION

S-225 S-226 S-227 S-228 S-229

STREAM ID	S-225	S-226	S-227	S-228	S-229
FROM :	P-203	M-204	HX-205	F-201	F-201
TO :	M-204	HX-205	F-201	----	P-204
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	5647.1601	5795.2158	5795.2158	144.8865	5650.3293
BTU/HR	-1.6570+07	-1.6605+07	-1.6791+07	-3.1649+04	-1.6759+07
SUBSTREAM: MIXED					
PHASE:	LIQUID	MIXED	MIXED	VAPOR	LIQUID
COMPONENTS: LBMOL/HR					
OXYGEN	8.5757-03	4.2400	4.2400	4.2334	6.6320-03
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	3.2778-06	1.4087-02	1.4087-02	1.4085-02	1.8974-06
AMMONIA	4.4005-03	4.6348-03	4.6348-03	7.7355-05	4.5574-03
WATER	121.9071	122.0399	122.0399	2.5620-02	122.0142
CARBO-01	6.3557-03	0.1690	0.1690	0.1612	7.8802-03
NIACINAM	27.6135	27.6135	27.6135	9.6211-08	27.6135
METDIAMI	2.9940-05	3.1198-05	3.1198-05	5.6141-07	3.0636-05
METHYLPI	0.2653	0.2846	0.2846	1.1209-02	0.2734
3-MET-01	0.2461	0.2536	0.2536	3.5164-03	0.2501
NICOT-01	0.2780	0.2789	0.2789	3.1750-04	0.2786
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	5.7046-05	2.7373-02	2.7373-02	0.9515	4.4082-05
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	2.1804-08	9.0944-05	9.0944-05	3.1656-03	1.2611-08
AMMONIA	2.9273-05	2.9921-05	2.9921-05	1.7386-05	3.0292-05
WATER	0.8109	0.7879	0.7879	5.7580-03	0.8110
CARBO-01	4.2278-05	1.0913-03	1.0913-03	3.6222-02	5.2378-05
NIACINAM	0.1837	0.1783	0.1783	2.1623-08	0.1835
METDIAMI	1.9916-07	2.0141-07	2.0141-07	1.2618-07	2.0363-07
METHYLPI	1.7647-03	1.8373-03	1.8373-03	2.5191-03	1.8171-03
3-MET-01	1.6373-03	1.6370-03	1.6370-03	7.9031-04	1.6620-03
NICOT-01	1.8493-03	1.8007-03	1.8007-03	7.1357-05	1.8518-03
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	0.2744	135.6763	135.6763	135.4641	0.2122
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	9.1823-05	0.3946	0.3946	0.3946	5.3152-05
AMMONIA	7.4944-02	7.8933-02	7.8933-02	1.3174-03	7.7615-02
WATER	2196.1913	2198.5821	2198.5821	0.4615	2198.1206
CARBO-01	0.2797	7.4396	7.4396	7.0928	0.3468
NIACINAM	3372.1641	3372.1643	3372.1643	1.1749-05	3372.1643
METDIAMI	3.4790-03	3.6252-03	3.6252-03	6.5236-05	3.5599-03
METHYLPI	26.3078	28.2227	28.2227	1.1116	27.1112
3-MET-01	22.9216	23.6143	23.6143	0.3275	23.2869
NICOT-01	28.9426	29.0392	29.0392	3.3055-02	29.0061
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	4.8593-05	2.3412-02	2.3412-02	0.9350	3.7558-05
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	1.6260-08	6.8096-05	6.8096-05	2.7233-03	9.4070-09

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 105
NIACIN PRODUCTION
STREAM SECTION

S-225 S-226 S-227 S-228 S-229 (CONTINUED)

STREAM ID	S-225	S-226	S-227	S-228	S-229
AMMONIA	1.3271-05	1.3620-05	1.3620-05	9.0927-06	1.3736-05
WATER	0.3889	0.3794	0.3794	3.1855-03	0.3890
CARBO-01	4.9531-05	1.2838-03	1.2838-03	4.8954-02	6.1378-05
NIACINAM	0.5971	0.5819	0.5819	8.1093-08	0.5968
METDIAMI	6.1607-07	6.2554-07	6.2554-07	4.5025-07	6.3004-07
METHYLPI	4.6586-03	4.8700-03	4.8700-03	7.6719-03	4.7982-03
3-MET-01	4.0590-03	4.0748-03	4.0748-03	2.2602-03	4.1213-03
NICOT-01	5.1252-03	5.0109-03	5.0109-03	2.2814-04	5.1335-03
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	150.3294	154.8983	154.8983	4.4494	150.4489
LB/HR	5647.1601	5795.2158	5795.2158	144.8865	5650.3293
CUFT/HR	76.3533	758.7494	913.9509	1563.2334	74.8273
STATE VARIABLES:					
TEMP F	77.2505	79.3753	32.0000	32.0000	32.0000
PRES PSIA	45.7298	37.7298	27.7298	15.0000	15.0000
VFRAC	0.0	2.8787-02	2.8529-02	1.0000	0.0
LFRAC	1.0000	0.9712	0.9715	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.1022+05	-1.0720+05	-1.0840+05	-7113.1518	-1.1139+05
BTU/LB	-2934.1894	-2865.2707	-2897.3321	-218.4418	-2966.0063
BTU/HR	-1.6570+07	-1.6605+07	-1.6791+07	-3.1649+04	-1.6759+07
ENTROPY:					
BTU/LBMOL-R	-53.7600	-52.1589	-54.4680	-0.7075	-56.0174
BTU/LB-R	-1.4311	-1.3941	-1.4559	-2.1726-02	-1.4916
DENSITY:					
LBMOL/CUFT	1.9689	0.2041	0.1695	2.8463-03	2.0106
LB/CUFT	73.9609	7.6379	6.3408	9.2684-02	75.5116
AVG MW	37.5652	37.4130	37.4130	32.5631	37.5565

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 106
NIACIN PRODUCTION
STREAM SECTION

S-230 S-231 S-301 S-302 S-303

STREAM ID	S-230	S-231	S-301	S-302	S-303
FROM :	P-204	HX-206	M-301	HX-301	DC-301
TO :	HX-206	M-301	HX-301	DC-301	N-301
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	5650.3293	5650.3293	2.5619+04	2.5619+04	0.0
BTU/HR	-1.6758+07	-1.6534+07	-1.5505+08	-1.5381+08	0.0
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	MIXED	MIXED	MISSING
COMPONENTS: LBMOL/HR					
OXYGEN	6.6320-03	6.6320-03	6.6531-03	6.6531-03	0.0
HYDROGEN	0.0	0.0	1.6566-16	1.6566-16	0.0
NITROGEN	1.8974-06	1.8974-06	7.4732-05	7.4732-05	0.0
AMMONIA	4.5574-03	4.5574-03	3.1469	3.1469	0.0
WATER	122.0142	122.0142	1227.4593	1227.4593	0.0
CARBO-01	7.8802-03	7.8802-03	8.3138-03	8.3138-03	0.0
NIACINAM	27.6135	27.6135	27.6135	27.6135	0.0
METDIAMI	3.0636-05	3.0636-05	3.0636-05	3.0636-05	0.0
METHYLPI	0.2734	0.2734	0.2734	0.2734	0.0
3-MET-01	0.2501	0.2501	0.2502	0.2502	0.0
NICOT-01	0.2786	0.2786	0.2786	0.2786	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	4.4082-05	4.4082-05	5.2843-06	5.2843-06	0.0
HYDROGEN	0.0	0.0	1.3157-19	1.3157-19	0.0
NITROGEN	1.2611-08	1.2611-08	5.9356-08	5.9356-08	0.0
AMMONIA	3.0292-05	3.0292-05	2.4995-03	2.4995-03	0.0
WATER	0.8110	0.8110	0.9749	0.9749	0.0
CARBO-01	5.2378-05	5.2378-05	6.6033-06	6.6033-06	0.0
NIACINAM	0.1835	0.1835	2.1932-02	2.1932-02	0.0
METDIAMI	2.0363-07	2.0363-07	2.4333-08	2.4333-08	0.0
METHYLPI	1.8171-03	1.8171-03	2.1713-04	2.1713-04	0.0
3-MET-01	1.6620-03	1.6620-03	1.9874-04	1.9874-04	0.0
NICOT-01	1.8518-03	1.8518-03	2.2129-04	2.2129-04	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	0.2122	0.2122	0.2129	0.2129	0.0
HYDROGEN	0.0	0.0	3.3394-16	3.3394-16	0.0
NITROGEN	5.3152-05	5.3152-05	2.0935-03	2.0935-03	0.0
AMMONIA	7.7615-02	7.7615-02	53.5941	53.5941	0.0
WATER	2198.1206	2198.1206	2.2113+04	2.2113+04	0.0
CARBO-01	0.3468	0.3468	0.3659	0.3659	0.0
NIACINAM	3372.1643	3372.1643	3372.1643	3372.1643	0.0
METDIAMI	3.5599-03	3.5599-03	3.5599-03	3.5599-03	0.0
METHYLPI	27.1112	27.1112	27.1112	27.1112	0.0
3-MET-01	23.2869	23.2869	23.3024	23.3024	0.0
NICOT-01	29.0061	29.0061	29.0061	29.0061	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	3.7558-05	3.7558-05	8.3100-06	8.3100-06	MISSING
HYDROGEN	0.0	0.0	1.3035-20	1.3035-20	MISSING
NITROGEN	9.4070-09	9.4070-09	8.1717-08	8.1717-08	MISSING

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 107
NIACIN PRODUCTION
STREAM SECTION

S-230 S-231 S-301 S-302 S-303 (CONTINUED)

STREAM ID	S-230	S-231	S-301	S-302	S-303
AMMONIA	1.3736-05	1.3736-05	2.0920-03	2.0920-03	MISSING
WATER	0.3890	0.3890	0.8632	0.8632	MISSING
CARBO-01	6.1378-05	6.1378-05	1.4282-05	1.4282-05	MISSING
NIACINAM	0.5968	0.5968	0.1316	0.1316	MISSING
METDIAMI	6.3004-07	6.3004-07	1.3896-07	1.3896-07	MISSING
METHYLPI	4.7982-03	4.7982-03	1.0583-03	1.0583-03	MISSING
3-MET-01	4.1213-03	4.1213-03	9.0958-04	9.0958-04	MISSING
NICOT-01	5.1335-03	5.1335-03	1.1322-03	1.1322-03	MISSING
AMMONICO	0.0	0.0	0.0	0.0	MISSING
TOTAL FLOW:					
LBMOL/HR	150.4489	150.4489	1259.0371	1259.0371	0.0
LB/HR	5650.3293	5650.3293	2.5619+04	2.5619+04	0.0
CUFT/HR	74.8355	76.8679	432.6425	464.6754	0.0
STATE VARIABLES:					
TEMP F	32.2422	90.0000	30.9724	77.0000	MISSING
PRES PSIA	45.0000	35.0000	35.0000	25.0000	MISSING
VFRAC	0.0	0.0	3.4792-04	2.6201-04	MISSING
LFRAC	1.0000	1.0000	0.9997	0.9997	MISSING
SFRAC	0.0	0.0	0.0	0.0	MISSING
ENTHALPY:					
BTU/LBMOL	-1.1138+05	-1.0990+05	-1.2315+05	-1.2216+05	MISSING
BTU/LB	-2965.7577	-2926.2048	-6052.0663	-6003.7353	MISSING
BTU/HR	-1.6758+07	-1.6534+07	-1.5505+08	-1.5381+08	MISSING
ENTROPY:					
BTU/LBMOL-R	-56.0060	-53.1487	-44.0519	-42.1344	MISSING
BTU/LB-R	-1.4912	-1.4152	-2.1649	-2.0707	MISSING
DENSITY:					
LBMOL/CUFT	2.0104	1.9572	2.9101	2.7095	MISSING
LB/CUFT	75.5033	73.5070	59.2147	55.1326	MISSING
AVG MW	37.5565	37.5565	20.3479	20.3479	MISSING

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 108
NIACIN PRODUCTION
STREAM SECTION

S-304 S-305 S-306 S-307 S-308

STREAM ID	S-304	S-305	S-306	S-307	S-308
FROM :	DC-301	N-301	P-301	HX-302	----
TO :	N-301	P-301	HX-302	DR-301	HX-303
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	2.5619+04	2.5619+04	2.5619+04	2.5619+04	30.8796
BTU/HR	-1.5381+08	-1.5381+08	-1.5381+08	-1.2488+08	-5.9364
SUBSTREAM: MIXED					
PHASE:	MIXED	MIXED	LIQUID	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
OXYGEN	6.6531-03	6.6531-03	6.6531-03	6.6531-03	0.0
HYDROGEN	1.6566-16	0.0	0.0	0.0	0.0
NITROGEN	7.4732-05	7.4732-05	7.4732-05	7.4732-05	1.1023
AMMONIA	3.1469	3.1469	3.1469	3.1469	0.0
WATER	1227.4593	1227.4593	1227.4593	1227.4593	0.0
CARBO-01	8.3138-03	8.3138-03	8.3138-03	8.3138-03	0.0
NIACINAM	27.6135	27.6135	27.6135	27.6135	0.0
METDIAMI	3.0636-05	3.0636-05	3.0636-05	3.0636-05	0.0
METHYLPI	0.2734	0.2734	0.2734	0.2734	0.0
3-MET-01	0.2502	0.2502	0.2502	0.2502	0.0
NICOT-01	0.2786	0.2786	0.2786	0.2786	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	5.2843-06	5.2843-06	5.2843-06	5.2843-06	0.0
HYDROGEN	1.3157-19	0.0	0.0	0.0	0.0
NITROGEN	5.9356-08	5.9356-08	5.9356-08	5.9356-08	1.0000
AMMONIA	2.4995-03	2.4995-03	2.4995-03	2.4995-03	0.0
WATER	0.9749	0.9749	0.9749	0.9749	0.0
CARBO-01	6.6033-06	6.6033-06	6.6033-06	6.6033-06	0.0
NIACINAM	2.1932-02	2.1932-02	2.1932-02	2.1932-02	0.0
METDIAMI	2.4333-08	2.4333-08	2.4333-08	2.4333-08	0.0
METHYLPI	2.1713-04	2.1713-04	2.1713-04	2.1713-04	0.0
3-MET-01	1.9874-04	1.9874-04	1.9874-04	1.9874-04	0.0
NICOT-01	2.2129-04	2.2129-04	2.2129-04	2.2129-04	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	0.2129	0.2129	0.2129	0.2129	0.0
HYDROGEN	3.3394-16	0.0	0.0	0.0	0.0
NITROGEN	2.0935-03	2.0935-03	2.0935-03	2.0935-03	30.8796
AMMONIA	53.5941	53.5941	53.5941	53.5941	0.0
WATER	2.2113+04	2.2113+04	2.2113+04	2.2113+04	0.0
CARBO-01	0.3659	0.3659	0.3659	0.3659	0.0
NIACINAM	3372.1643	3372.1643	3372.1643	3372.1643	0.0
METDIAMI	3.5599-03	3.5599-03	3.5599-03	3.5599-03	0.0
METHYLPI	27.1112	27.1112	27.1112	27.1112	0.0
3-MET-01	23.3024	23.3024	23.3024	23.3024	0.0
NICOT-01	29.0061	29.0061	29.0061	29.0061	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	8.3100-06	8.3100-06	8.3100-06	8.3100-06	0.0
HYDROGEN	1.3035-20	0.0	0.0	0.0	0.0
NITROGEN	8.1717-08	8.1717-08	8.1717-08	8.1717-08	1.0000

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 109
NIACIN PRODUCTION
STREAM SECTION

S-304 S-305 S-306 S-307 S-308 (CONTINUED)

STREAM ID	S-304	S-305	S-306	S-307	S-308
AMMONIA	2.0920-03	2.0920-03	2.0920-03	2.0920-03	0.0
WATER	0.8632	0.8632	0.8632	0.8632	0.0
CARBO-01	1.4282-05	1.4282-05	1.4282-05	1.4282-05	0.0
NIACINAM	0.1316	0.1316	0.1316	0.1316	0.0
METDIAMI	1.3896-07	1.3896-07	1.3896-07	1.3896-07	0.0
METHYLPI	1.0583-03	1.0583-03	1.0583-03	1.0583-03	0.0
3-MET-01	9.0958-04	9.0958-04	9.0958-04	9.0958-04	0.0
NICOT-01	1.1322-03	1.1322-03	1.1322-03	1.1322-03	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	1259.0371	1259.0371	1259.0371	1259.0371	1.1023
LB/HR	2.5619+04	2.5619+04	2.5619+04	2.5619+04	30.8796
CUFT/HR	496.3740	556.2393	400.4598	3.8057+05	215.1855
STATE VARIABLES:					
TEMP F	77.0265	77.0000	76.9392	392.0000	77.0000
PRES PSIA	20.0000	15.0000	39.9465	29.9465	29.5007
VFRAC	3.0069-04	3.5328-04	0.0	1.0000	1.0000
LFRAC	0.9997	0.9996	1.0000	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.2216+05	-1.2216+05	-1.2216+05	-9.9190+04	-5.3854
BTU/LB	-6003.7353	-6003.7935	-6003.6296	-4874.6840	-0.1922
BTU/HR	-1.5381+08	-1.5381+08	-1.5381+08	-1.2488+08	-5.9364
ENTROPY:					
BTU/LBMOL-R	-42.1335	-42.1348	-42.1328	-9.4357	-1.3937
BTU/LB-R	-2.0707	-2.0707	-2.0706	-0.4637	-4.9752-02
DENSITY:					
LBMOL/CUFT	2.5365	2.2635	3.1440	3.3083-03	5.1226-03
LB/CUFT	51.6119	46.0571	63.9734	6.7316-02	0.1435
AVG MW	20.3479	20.3479	20.3479	20.3479	28.0135

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 110
NIACIN PRODUCTION
STREAM SECTION

S-309 S-310 S-311 S-312 S-312A

STREAM ID	S-309	S-310	S-311	S-312	S-312A
FROM :	HX-303	DR-301	C-301	HX-304B	HX-304A
TO :	DR-301	C-301	HX-304A	F-301	HX-304B
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
TOTAL STREAM:					
LB/HR	30.8796	2.2481+04	2.2481+04	2.2481+04	2.2481+04
BTU/HR	2425.2806	-1.2457+08	-1.1920+08	-1.5381+08	-1.5206+08
SUBSTREAM: MIXED					
PHASE:	VAPOR	VAPOR	VAPOR	MIXED	MIXED
COMPONENTS: LBMOL/HR					
OXYGEN	0.0	6.6320-02	6.6320-02	6.6320-02	6.6320-02
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	1.1023	11.0231	11.0231	11.0231	11.0231
AMMONIA	0.0	3.1484	3.1484	3.1484	3.1484
WATER	0.0	1227.4695	1227.4695	1227.4695	1227.4695
CARBO-01	0.0	7.8802-02	7.8802-02	7.8802-02	7.8802-02
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	0.0	0.0	0.0	0.0
METHYLPI	0.0	0.0	0.0	0.0	0.0
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	0.0	5.3407-05	5.3407-05	5.3407-05	5.3407-05
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	1.0000	8.8768-03	8.8768-03	8.8768-03	8.8768-03
AMMONIA	0.0	2.5354-03	2.5354-03	2.5354-03	2.5354-03
WATER	0.0	0.9885	0.9885	0.9885	0.9885
CARBO-01	0.0	6.3459-05	6.3459-05	6.3459-05	6.3459-05
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	0.0	0.0	0.0	0.0
METHYLPI	0.0	0.0	0.0	0.0	0.0
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	0.0	2.1222	2.1222	2.1222	2.1222
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	30.8796	308.7963	308.7963	308.7963	308.7963
AMMONIA	0.0	53.6188	53.6188	53.6188	53.6188
WATER	0.0	2.2113+04	2.2113+04	2.2113+04	2.2113+04
CARBO-01	0.0	3.4681	3.4681	3.4681	3.4681
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	0.0	0.0	0.0	0.0
METHYLPI	0.0	0.0	0.0	0.0	0.0
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	0.0	9.4398-05	9.4398-05	9.4398-05	9.4398-05
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	1.0000	1.3736-02	1.3736-02	1.3736-02	1.3736-02

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 111
NIACIN PRODUCTION
STREAM SECTION

S-309 S-310 S-311 S-312 S-312A (CONTINUED)

STREAM ID	S-309	S-310	S-311	S-312	S-312A
AMMONIA	0.0	2.3850-03	2.3850-03	2.3850-03	2.3850-03
WATER	0.0	0.9836	0.9836	0.9836	0.9836
CARBO-01	0.0	1.5427-04	1.5427-04	1.5427-04	1.5427-04
NIACINAM	0.0	0.0	0.0	0.0	0.0
METDIAMI	0.0	0.0	0.0	0.0	0.0
METHYLPI	0.0	0.0	0.0	0.0	0.0
3-MET-01	0.0	0.0	0.0	0.0	0.0
NICOT-01	0.0	0.0	0.0	0.0	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	1.1023	1241.7861	1241.7861	1241.7861	1241.7861
LB/HR	30.8796	2.2481+04	2.2481+04	2.2481+04	2.2481+04
CUFT/HR	516.9630	7.7489+05	2.6283+05	1364.9568	1440.1101
STATE VARIABLES:					
TEMP F	392.0000	387.1028	887.2012	32.0000	100.0000
PRES PSIA	19.5007	14.5007	68.0082	58.0082	63.0082
VFRAC	1.0000	1.0000	1.0000	9.0036-03	9.1074-03
LFRAC	0.0	0.0	0.0	0.9910	0.9909
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	2200.1776	-1.0032+05	-9.5989+04	-1.2386+05	-1.2245+05
BTU/LB	78.5400	-5541.1690	-5302.0945	-6841.8061	-6763.8642
BTU/HR	2425.2806	-1.2457+08	-1.1920+08	-1.5381+08	-1.5206+08
ENTROPY:					
BTU/LBMOL-R	2.6614	-6.6712	-5.7237	-42.3579	-39.6719
BTU/LB-R	9.5003-02	-0.3685	-0.3162	-2.3397	-2.1913
DENSITY:					
LBMOL/CUFT	2.1323-03	1.6025-03	4.7246-03	0.9098	0.8623
LB/CUFT	5.9733-02	2.9012-02	8.5534-02	16.4703	15.6108
AVG MW	28.0135	18.1039	18.1039	18.1039	18.1039

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 112
NIACIN PRODUCTION
STREAM SECTION

S-313 S-314 S-315 S-316 S-317

STREAM ID	S-313	S-314	S-315	S-316	S-317
FROM :	F-301	SP-302	SP-302	DR-301	F-301
TO :	SP-302	----	DR-301	----	SP-301
CLASS:	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
MAX CONV. ERROR:	-9.9363-09	0.0	0.0	0.0	4.7926-11
TOTAL STREAM:					
LB/HR	314.5922	31.4592	283.1330	3451.5876	2.2167+04
BTU/HR	-1.8108+04	-1810.8064	-1.6297+04	-1.1762+06	-1.5379+08
SUBSTREAM: MIXED					
PHASE:	VAPOR	VAPOR	VAPOR	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
OXYGEN	6.6297-02	6.6297-03	5.9667-02	0.0	2.3426-05
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	11.0231	1.1023	9.9207	0.0	8.0927-05
AMMONIA	1.6058-03	1.6058-04	1.4452-03	0.0	3.1468
WATER	1.1241-02	1.1241-03	1.0117-02	0.0	1227.4582
CARBO-01	7.8320-02	7.8320-03	7.0488-02	0.0	4.8173-04
NIACINAM	0.0	0.0	0.0	27.6135	0.0
METDIAMI	0.0	0.0	0.0	3.0636-05	0.0
METHYLPI	0.0	0.0	0.0	0.2734	0.0
3-MET-01	0.0	0.0	0.0	0.2502	0.0
NICOT-01	0.0	0.0	0.0	0.2786	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MOLE FRAC					
OXYGEN	5.9297-03	5.9297-03	5.9297-03	0.0	1.9036-08
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.9859	0.9859	0.9859	0.0	6.5762-08
AMMONIA	1.4363-04	1.4363-04	1.4363-04	0.0	2.5571-03
WATER	1.0054-03	1.0054-03	1.0054-03	0.0	0.9974
CARBO-01	7.0051-03	7.0051-03	7.0051-03	0.0	3.9145-07
NIACINAM	0.0	0.0	0.0	0.9718	0.0
METDIAMI	0.0	0.0	0.0	1.0781-06	0.0
METHYLPI	0.0	0.0	0.0	9.6207-03	0.0
3-MET-01	0.0	0.0	0.0	8.8056-03	0.0
NICOT-01	0.0	0.0	0.0	9.8047-03	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
OXYGEN	2.1214	0.2121	1.9093	0.0	7.4959-04
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	308.7940	30.8794	277.9146	0.0	2.2670-03
AMMONIA	2.7348-02	2.7348-03	2.4613-02	0.0	53.5914
WATER	0.2025	2.0251-02	0.1823	0.0	2.2113+04
CARBO-01	3.4469	0.3447	3.1022	0.0	2.1201-02
NIACINAM	0.0	0.0	0.0	3372.1643	0.0
METDIAMI	0.0	0.0	0.0	3.5599-03	0.0
METHYLPI	0.0	0.0	0.0	27.1112	0.0
3-MET-01	0.0	0.0	0.0	23.3024	0.0
NICOT-01	0.0	0.0	0.0	29.0061	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
COMPONENTS: MASS FRAC					
OXYGEN	6.7434-03	6.7434-03	6.7434-03	0.0	3.3816-08

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 113
NIACIN PRODUCTION
STREAM SECTION

S-313 S-314 S-315 S-316 S-317 (CONTINUED)

STREAM ID	S-313	S-314	S-315	S-316	S-317
HYDROGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.9816	0.9816	0.9816	0.0	1.0227-07
AMMONIA	8.6932-05	8.6932-05	8.6932-05	0.0	2.4177-03
WATER	6.4371-04	6.4371-04	6.4371-04	0.0	0.9976
CARBO-01	1.0957-02	1.0957-02	1.0957-02	0.0	9.5642-07
NIACINAM	0.0	0.0	0.0	0.9770	0.0
METDIAMI	0.0	0.0	0.0	1.0314-06	0.0
METHYLPI	0.0	0.0	0.0	7.8547-03	0.0
3-MET-01	0.0	0.0	0.0	6.7512-03	0.0
NICOT-01	0.0	0.0	0.0	8.4037-03	0.0
AMMONICO	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	11.1805	1.1181	10.0625	28.4158	1230.6056
LB/HR	314.5922	31.4592	283.1330	3451.5876	2.2167+04
CUFT/HR	1015.6803	122.6666	1103.9997	44.4549	349.2765
STATE VARIABLES:					
TEMP F	32.0000	31.6692	31.6692	387.1028	32.0000
PRES PSIA	58.0082	48.0082	48.0082	14.5007	58.0082
VFRAC	1.0000	1.0000	1.0000	0.0	0.0
LFRAC	0.0	0.0	0.0	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1619.6091	-1619.6091	-1619.6091	-4.1394+04	-1.2497+05
BTU/LB	-57.5604	-57.5604	-57.5604	-340.7833	-6938.0891
BTU/HR	-1.8108+04	-1810.8064	-1.6297+04	-1.1762+06	-1.5379+08
ENTROPY:					
BTU/LBMOL-R	-3.1976	-2.8223	-2.8223	-97.5291	-42.7137
BTU/LB-R	-0.1136	-0.1003	-0.1003	-0.8029	-2.3713
DENSITY:					
LBMOL/CUFT	1.1008-02	9.1146-03	9.1146-03	0.6392	3.5233
LB/CUFT	0.3097	0.2565	0.2565	77.6425	63.4644
AVG MW	28.1375	28.1375	28.1375	121.4673	18.0128

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 114
NIACIN PRODUCTION
STREAM SECTION

S-318 S-319

STREAM ID	S-318	S-319
FROM :	SP-301	SP-301
TO :	M-301	----
CLASS:	MIXCIPSD	MIXCIPSD
TOTAL STREAM:		
LB/HR	1.9950+04	2216.6619
BTU/HR	-1.3841+08	-1.5379+07
SUBSTREAM: MIXED		
PHASE:	MIXED	MIXED
COMPONENTS: LBMOL/HR		
OXYGEN	2.1083-05	2.3426-06
HYDROGEN	0.0	0.0
NITROGEN	7.2834-05	8.0927-06
AMMONIA	2.8321	0.3147
WATER	1104.7124	122.7458
CARBO-01	4.3355-04	4.8173-05
NIACINAM	0.0	0.0
METDIAMI	0.0	0.0
METHYLPI	0.0	0.0
3-MET-01	0.0	0.0
NICOT-01	0.0	0.0
AMMONICO	0.0	0.0
COMPONENTS: MOLE FRAC		
OXYGEN	1.9036-08	1.9036-08
HYDROGEN	0.0	0.0
NITROGEN	6.5762-08	6.5762-08
AMMONIA	2.5571-03	2.5571-03
WATER	0.9974	0.9974
CARBO-01	3.9145-07	3.9145-07
NIACINAM	0.0	0.0
METDIAMI	0.0	0.0
METHYLPI	0.0	0.0
3-MET-01	0.0	0.0
NICOT-01	0.0	0.0
AMMONICO	0.0	0.0
COMPONENTS: LB/HR		
OXYGEN	6.7463-04	7.4959-05
HYDROGEN	0.0	0.0
NITROGEN	2.0403-03	2.2670-04
AMMONIA	48.2323	5.3591
WATER	1.9902+04	2211.3003
CARBO-01	1.9081-02	2.1201-03
NIACINAM	0.0	0.0
METDIAMI	0.0	0.0
METHYLPI	0.0	0.0
3-MET-01	0.0	0.0
NICOT-01	0.0	0.0
AMMONICO	0.0	0.0
COMPONENTS: MASS FRAC		
OXYGEN	3.3816-08	3.3816-08
HYDROGEN	0.0	0.0
NITROGEN	1.0227-07	1.0227-07

ASPEN PLUS PLAT: WIN32 VER: 25.0 03/27/2013 PAGE 115
NIACIN PRODUCTION
STREAM SECTION

S-318 S-319 (CONTINUED)

STREAM ID	S-318	S-319
AMMONIA	2.4177-03	2.4177-03
WATER	0.9976	0.9976
CARBO-01	9.5642-07	9.5642-07
NIACINAM	0.0	0.0
METDIAMI	0.0	0.0
METHYLPI	0.0	0.0
3-MET-01	0.0	0.0
NICOT-01	0.0	0.0
AMMONICO	0.0	0.0
TOTAL FLOW:		
LBMOL/HR	1107.5450	123.0606
LB/HR	1.9950+04	2216.6619
CUFT/HR	314.3547	34.9283
STATE VARIABLES:		
TEMP F	32.0274	32.0274
PRES PSIA	48.0082	48.0082
VFRAC	1.1579-08	1.1579-08
LFRAC	1.0000	1.0000
SFRAC	0.0	0.0
ENTHALPY:		
BTU/LBMOL	-1.2497+05	-1.2497+05
BTU/LB	-6938.0891	-6938.0891
BTU/HR	-1.3841+08	-1.5379+07
ENTROPY:		
BTU/LBMOL-R	-42.7123	-42.7123
BTU/LB-R	-2.3712	-2.3712
DENSITY:		
LBMOL/CUFT	3.5232	3.5232
LB/CUFT	63.4632	63.4632
AVG MW	18.0128	18.0128

```
ASPEN PLUS   PLAT: WIN32     VER: 25.0                  03/27/2013  PAGE 116
                              NIACIN PRODUCTION
                             PROBLEM STATUS SECTION

BLOCK STATUS
------------

****************************************************************************
*                                                                          *
* Calculations were completed normally                                     *
*                                                                          *
* All Unit Operation blocks were completed normally                        *
*                                                                          *
* All streams were flashed normally                                        *
*                                                                          *
* All Convergence blocks were completed normally                           *
*                                                                          *
****************************************************************************
```

D. SAMPLE DESIGN AND COST CALCULATIONS

Reaction 1	**Exothermic**					**Percent Difference**	**%**		**Energy Balance**		
Chemical	MPDA	Al_2O_3 (catalyst)	3-Methylpiperidine	NH_3	**START (kg)**	Reaction 1	1.26319E-14		-17885689.73	KJ/hr	
Mass of Chemical (kg/hr)	1800				1800	Reaction 2	0.019965715				
Moles/hr	15490.53356					Side Reaction	0.00042398		**Reactions 1 & 2**		
Molecular Weight (kg/mol)	0.1162	0.10196	0.09917	0.01703		Reaction 3	0.04444866		2523985.234	KJ/hr	
Stoichiometry	-1	0	1	1		Reaction 4	0.007810288				
Fractional Conversion	0.99					Side Reaction	0				
Final Moles/hr	154.9053356		15335.62823	15335.62823	**END (kg)**						
Final Mass (kg/hr)	18		1520.834251	261.1657487	1800						
*ΔH_f (KJ/mol*hr)*	-106.43	--	-96.59	-45.92	**Energy (KJ/hr)**						
Overall Conversion	0.99				-553309.4664						
Reaction 2	**Endothermic**					**Side Reaction**	**Exothermic**				
Chemical	Methyl Piperidine	Pd/A_2O_3 (catalyst)	3-Picoline	H_2	**START (kg)**	3-Picoline	O_2	N_2	CO_2	H_2O	**START (kg)**
Mass of Chemical (kg/hr)	1520.834251				1520.834251	1413.924986	376.5203442				1790.44533
Moles/hr	15335.62823					15182.27194	11766.26076				
Molecular Weight (kg/mol)	0.09917	N/A	0.09313	0.00202		0.09313	0.032	0.02801	0.04401	0.01802	
Stoichiometry	-1	0	1	3		-2	-15.5	1	12	7	
Fractional Conversion	0.99					0.1					
Final Moles/hr	153.3562823		15182.27194	45546.81583	**END (kg)**	13664.04475	0	759.1135972	9109.363167	5313.795181	**END (kg)**
Final Mass (kg/hr)	15.20834251	--	1413.924986	92.00456799	1521.137897	1272.532488	0	21.26277186	400.903073	95.75458916	1790.452922
*ΔH_f (KJ/mol*hr)*	-96.59		106.1	0	**Energy (KJ/hr)**	106.1	0	0	-393.509	-241.818	**Energy (KJ/hr)**
Overall Conversion	**0.88209**				3077294.701	**0.793881**					-5030671.619
Reaction 3	1:1.5:1 to 1:2.5:4 ratio	**Add Oxygen**	**Add Ammonia**								
Chemical	3-Picoline	O_2	NH_3	Al_2O_3 (catalyst)	3-Cyanopyridine	H_2O	**START (kg)**				
Mass of Chemical (kg/hr)	1272.532488	655.874148	232.6986821				2161.105318				
Moles/hr	13664.04475	20496.06713	13664.04475								
Molecular Weight (kg/mol)	0.09917	0.032	0.01703	0.10196	0.10411	0.01802					
Stoichiometry	-1	-1.5	-1	0	1	3					
Fractional Conversion	0.99										
Final Moles/hr	136.6404475	204.9606713	136.6404475	0	13527.4043	40582.21291	**END (kg)**				
Final Mass (kg/hr)	13.55063318	6.55874148	2.326986821	0	1408.338062	731.2914766	2162.0659				
*ΔH_f (KJ/mol*hr)*	106.1	0	-45.92	--	274.77	-241.818	**Energy (KJ/hr)**				
Overall Conversion	**0.78594219**						-6910663.872				
Reaction 4		**Add Water**			**Side Reaction**	**Add Water**					
Chemical	3-Cyanopyridine	H_2O (basic)	Nicotinamide	**START (kg)**	Nicotinamide	H_2O (basic)	Niacin	NH_3	**START (kg)**		
Mass of Chemical (kg/hr)	1408.338062	306.34		1714.678062	1635.446947	270.3			1905.746947		
Moles/hr	13527.4043	17000			13392.13026	15000					
Molecular Weight (kg/mol)	0.10411	0.01802	0.12212		0.12212	0.01802	0.12311	0.01703			
Stoichiometry	-1	-1	1		-1	-1	1	1			
Fractional Conversion	0.99				0.9						
Final Moles/hr	135.274043	3607.86974	13392.13026	**END (kg)**	1339.213026	2947.082766	12052.91723	12052.91723	**END (kg)**		
Final Mass (kg/hr)	14.08338062	65.01381272	1635.446947	1714.544141	163.5446947	53.10643144	1483.834641	205.2611805	1905.746947		
*ΔH_f (KJ/mol*hr)*	274.77	--	-58.29	**Energy (KJ/hr)**	-58.29	--	-344.9	-45.92	**Energy (KJ/hr)**		
Overall Conversion	**0.778082768**			-4460382.904	**0.700274491**				-4007956.568		

Sample Catalyst Regeneration Oxygen Flow Calculations (R-101)

Based on the relative low concentration of hydrocarbons in our process streams and lacking data from any of the patents, it was assumed that catalysts in reactors R101 and R201 would need regenerating every 6 months via oxidation to remove coke buildup. It was also assumed that the carbon building up at the end of 6 months is equivalent to 3% of the catalysts original weight.
$m_{catalyst}$ = 5,600 lbs = 2,540 kg

$$n_{carbon} = \frac{(0.03)(M_{catalyst})}{MW_{carbon}} = \frac{(0.03)(2540\,kg)}{12.01\frac{kg}{kmol}} = 6.35 \text{ kmol} = n_{oxygen}$$

Given the 1:1 ratio of C to O_2 molecules in the typical combustion reaction

$$C + O_2 \rightarrow CO_2$$

$m_{oxygen} = (n_{oxygen}) * (MW_{oxygen})$ = (6.35)(16.00 kg/kmol) = 203 kg = **448 lbs/6 months**

Any heat given off during the combustion will be borne away by the cooling fluid within each reactor. Additionally, the CO_2 that is produced is sent to a wet scrubber to prevent pollution.

Sample Catalyst Price Calculations (R-101)

For the first reactor, the mass of HZSM-5 catalyst required, $m_{catalyst}$ for the entire reactor train = 5,600 lb

Assuming a catalyst density of 50 lb/ft^3 and a void fraction, ϵ of 0.5, the total volume of catalysts required:

$$V_{catalyst} = \left(\frac{m_{catalyst}}{\rho_{catalyst}}\right) \div \epsilon = \left(\frac{5600\ \text{lb}}{50\ \frac{\text{lb}}{\text{ft}^3}}\right) \div (0.5) = 224\ \text{ft}^3$$

Cost

The price, $P_{catalyst}$ of the ZSM-5 catalyst was estimated as follows:

$$P_{catalyst} = m_{catalyst} \times \sum P_i \times x_i \text{ where i the element in the catalyst}$$

The β-zeolite has a chemical formula of $Na_nAl_nSi_{96-n}O_{192}$ (0<n<27). To get Si/Al = 18 as specified in the patent, n = 5,

Element	x	Price ($/lb)	(P)(x/x_{total})($/lb)
Na	10	0.45	0.01
Al	10	0.86	0.01
Si	86	0.94	0.29
O	192	0.56	0.37
	x_{total} =298		$\sum P_i \times \frac{x_i}{x_{total}} = 0.68$

$$P_{catalyst} = 5600\ \text{lb} \times \$\ 0.68\ /\text{lb} = \$3,808$$

Sample Catalyst Price Calculations (R-102)

For the second reactor, the mass of 1% Pd-SiO_2/Al_2O_3 catalyst required, $m_{catalyst}$ for the entire reactor train = 6,410 lb

To calculate the catalyst density, the density of each compound (Pd, SiO_2, and Al_2O_3) was weighted against its mass fraction:

$$\rho_{catalyst} = \sum \rho_i \times x_i = \left(0.01 \times 12.023\frac{g}{cm^3} + 0.495 \times 2.65\frac{g}{cm^3} + 0.495 \times 2.65\frac{g}{cm^3}\right) = 3.39\frac{g}{cm^3}$$
$$= 211.5\frac{lb}{ft^3}$$

With a weighted catalyst density of 211 lb/ft^3 and a void fraction, ϵ of 0.5, the total volume of catalysts required:

$$V_{catalyst} = \left(\frac{m_{catalyst}}{\rho_{catalyst}}\right) \div \epsilon = \left(\frac{6410\text{ lb}}{211.5\ \frac{lb}{ft^3}}\right) \div (0.5) = 60\text{ ft}^3$$

Cost

The price, $P_{catalyst}$ of the 1% Pd-SiO_2/Al_2O_3 catalyst was estimated as follows:

$$P_{catalyst} = m_{catalyst} \times \sum P_i \times x_i \text{ where i the element in the catalyst}$$

Compound	**x**	**Price ($/lb)**	**(P)(x/x_{total})($/lb)**
Pd	0.01	12144	121.44
SiO_2	0.495	0.64	0.31
Al_2O_3	0.495	0.91	0.45
			$\sum P_i \times \frac{x_i}{x_{total}} = 122.20$

$$P_{catalyst} = 6{,}410\text{ lb} \times \$\ 122.20/\text{lb} = \$783{,}300$$

Sample Catalyst Price Calculations (R-201)

For the third reactor, the mass and price of catalyst are calculated by sourcing bulk prices for the different catalysts required. The overall results are shown below:

Compound	V_2O_5	TiO_2	ZrO_2	MoO_3
Mass (lb)	90,548	39,761	61,344	71,660
Price per lb ($/lb)	6.22	4.70	4.00	9.07
Price ($)	563,166	186,877	245,375	650,089

$P_{\text{catalyst}} = \$1{,}645{,}510$

Sample Catalyst Price Calculations (R-202A, B, C)

The fourth reaction train consists of three reactor vessels in a continuous cascade. Each vessel has a volume, V of 6,975 ft^3. It was determined that each 6,975 ft^3 tank would house 1,740 lb (dry weight) of the whole cell biocatalyst *R. rhodochrous* J1 immobilized in polyacrylamide particles.

Cell density in each vessel would then be:

$$\rho_{\text{cell}} = \frac{\text{mass of cells (lb)}}{\text{volume of vessel (ft}^3)} = \frac{1740\text{ lb}}{6975\text{ ft}^3} = 0.25\,\frac{\text{lb}}{\text{ft}^3}$$

Cost

For each vessel, 1,740 lb (dry weight) of the whole cell biocatalyst *R. rhodochrous* J1 immobilized in polyacrylamide (PAM) particles is required. The biocatalyst produced by *R. rhodochrous* J1 that is responsible for the reaction is nitrile hydratase, NHase.

The price for the biocatalyst in bulk quantities was not obtainable (Dia-Nitrix Co., Ltd sells it but the authors were unable to obtain a price quote from them); therefore, cost estimation methods were used to estimate the price of the biocatalyst.

Assuming that each polyacrylamide-*R. rhodochrous* particle consists of equal percentage by mass of either substance—50 mass% of PAM and 50 mass% of *R. rhodochrous.* Another assumption made is that only 1% of the *R. rhodochrous* whole cells is the actual enzyme, NHase. This means that using immobilized enzyme instead of whole cells, 870 lb of PAM and 8.7 lb of NHase would be required, giving a total of 878.7 lb.

Keeping as the foundation the retail price (provided by Sigma-Aldrich), the price for each chemical goes through a fluctuation of price proportionate to the bulk purchase, i.e. the cost on a commercial level, is much cheaper compared to the cost for chemicals for lab-scale purposes, which are purchased in small amounts and with a higher price fluctuation. On a lab scale, the prices (from http://www.sigmaaldrich.com/) are as follows:

Price of PAM = $130/ 25 g = $2,359/lb

Price of NHase = $188/ 50 mg = $1,705,510/lb

While the prices of both these chemicals are very high, there is evidence that a bulk market for both these products exists. Bulk prices for PAM are listed at \$1.2/lb. This is a scaling ratio of (2359/1.2) = 1,966 ≅ 2,000. Since both PAM and NHase are usually used for biologics purposes, as opposed to as commodity chemicals, it would be safe to assume that they would scale the same way. Thus, the price of NHase was converted to an estimated bulk quantity price using a price correlation factor and a scaling factor of ~0.75 (Dieudonné, B., et al., 2012).

$$\text{Price of NHase} = \frac{\$1{,}705{,}510}{\text{lb}} \times \left(\frac{2{,}359}{1.2}\right)^{0.75} = \frac{\$5{,}777}{\text{lb}}$$

This price is a conservatively high estimate (more than 3 times the upper bound) according to "Guidelines and Cost Analysis for Catalyst Production in Biocatalytic Processes" that gives the range of free enzyme price as \$690/lb to \$1,725/lb based on "typical values of biocatalyst cost" (Tufvesson, P., et al., 2010). However, the paper also states that the immobilization process "increases the specific enzyme cost by a factor of 4." This would put our estimate price of enzyme inside that price range.

Compound	PAM	NHase	Total
Mass (lb)	870	8.7	
Price per lb (\$/lb)	1.2	5776.89	
Price (\$)	1,044	50,259	51,303

This means that the total price per lb of biocatalyst = $\frac{\$51{,}303}{(870+8.7)\text{ lb}} = \frac{\$175}{\text{lb}}$

This sits well in the range of immobilized enzyme price of \$69/lb to \$690/lb given in "Guidelines and Cost Analysis for Catalyst Production in Biocatalytic Processes," making it a confident estimate.

For all three vessels, the total price of biocatalyst is \$153,910.

Sample Adsorbent (Activated Carbon) Calculations (DC-301)

Adsorbent (Activated Carbon)
Applicable Block: DC-301

Variable		Description	Unit
S	=	Size Factor = Bulk volume	ft^3

Relevant Equations: **Source**

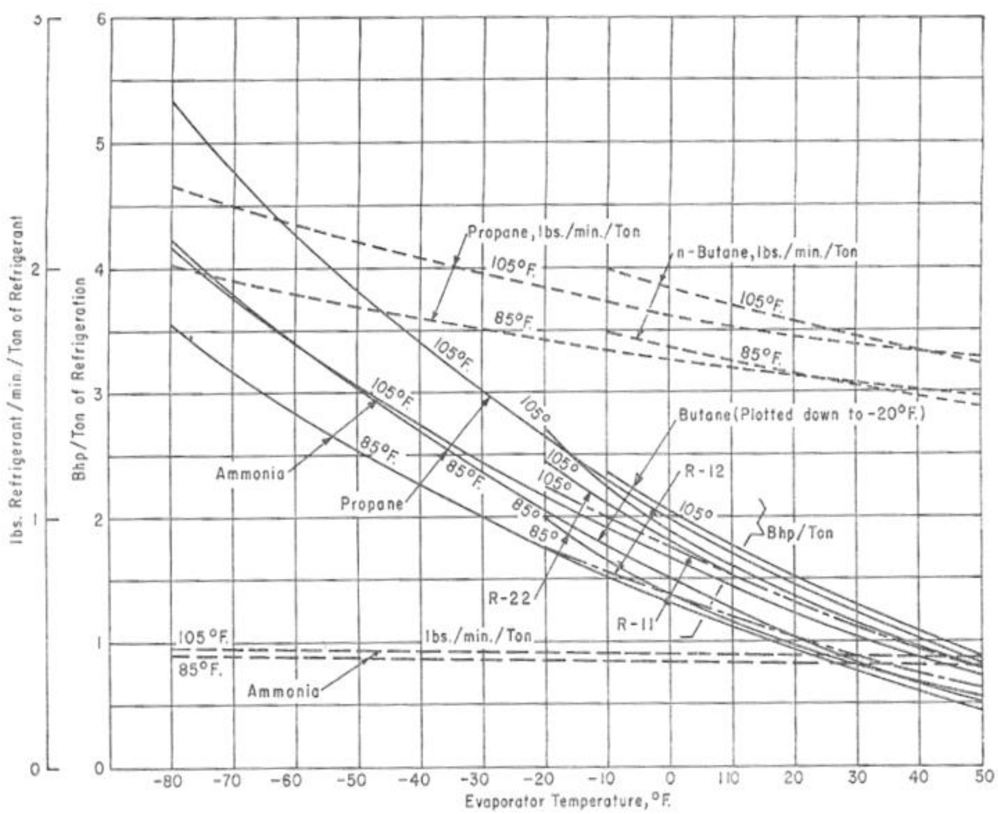
1) Find Cost

C_P = $30 \times S$ SSLW (T22.32)

C_P = $(575.4/500) * C_p$ (CE=575.4)

Refrigeration Power Requirements Chart

Chart used to calculate the electricity needed for refrigeration units. -120°F needs about 7 hp per ton of refrigeration.



Source: Ludwig. P.E, E. E. (2001). Chapter 11 Refrigeration systems. Applied Process Design for Chemical & Petrochemical Plants. E. E. Ludwig. P.E, Gulf Professional Publishing. ***Volume 3:*** *289-367.*

Sample Calculations: Dowtherm System

To effectively calculate the cost of the Dowtherm system used in the process, costing for a furnace, pump, and Dowtherm A was taken from a previous report, *Hydrogenation of Maleic Anhydride Tetrahydrofuran.* In the report from 2009, a total of 11,349 lbs of Dowtherm A were used for 17,038,956 BTU/hr needed for heat transfer. 68,093 lbs/hr were needed. Therefore, the heating capacity of a pound of Dowtherm A was calculated as

$$\frac{17{,}038{,}956\,\frac{\text{BTU}}{\text{hr}}}{68093\,\frac{\text{lbs}}{\text{hr}}} = 250\,\frac{\text{BTU}}{\text{lb}}$$

For the overall cost of the furnace and the pump, a cost of $700,000 for a furnace that has the capacity for 17 MMBTU/hr. The pump cost $6,900 to have the capacity listed above. Dowtherm A, as quoted from a Dow representative, is around $4.68/lb in 2009. To convert to our process, a factor was calculated to scale down the cost and flow rate of the Dowtherm.

$$\frac{17{,}038{,}956\,\frac{\text{BTU}}{\text{hr}}}{6{,}963{,}000\,\frac{\text{BTU}}{\text{hr}}} = 0.408$$

This factor was used to scale the costing for the pump and furnace.

$$Pump\ Cost: \$6{,}900 * 0.408 = \$2{,}819.34$$

$$Furnace\ Cost: \$700{,}000 * 0.408 = \$286{,}020$$

However, since this was calculated in 2009 when the CE was 521, these costs needed to be scaled up.

$$\text{Pump Cost}: \$2{,}819.34 * \left(\frac{570}{521}\right) = \$3{,}035$$

$$\text{Furnace Cost}: \$286{,}020 * \left(\frac{570}{521}\right) = \$312{,}920$$

It was then calculated how much Dowtherm A was needed for our process assuming that the heating value is 250 BTU/hr. The overall cost of the Dowtherm was also calculated, assuming the Dowtherm is pumped constantly in the system. A factor of 1/6th was used to find the total amount of Dowtherm necessary to be put into the system. CE factors were also taken into account to deal with inflation.

$$\frac{6{,}963{,}000\,\frac{\text{BTU}}{\text{hr}}}{250\,\frac{\text{BTU}}{\text{hr}}} = 27{,}852\ \text{lb/hr}$$

$$27{,}852\,\frac{\text{lb}}{\text{hr}} * \frac{1\ \text{hr}}{6} * \frac{\$4.68}{\text{lb}} * \left(\frac{570}{521}\right) = \$23{,}767$$

Final cost calculations also take into consideration total bare module cost. For a furnace, 2.2 is used whereas 3.30 is used for a pump.

$$\text{Pump Cost}: \$3{,}035 * 3.3 = \$10{,}016$$

$$\text{Furnace Cost}: \$312{,}920 * 2.2 = \$688{,}424$$

Overall, the cost for the entire Dowtherm A system, including the furnace, pump, and Dowtherm A chemical is $722,207.

Sample Calculations: Distillation or Absorbing Column

<u>Tower:</u>
All of the data used in these calculations were taken from the ASPEN report for the distillation column. The top stage conditions were used to calculate the flooding velocity and the final diameter of the column itself. This distillation column was defined by the authors to have sieve trays and a tray spacing of 12 inches to make sure that the column was only one unit and did not have to separated into two distillation columns in series. From ASPEN, the number of trays calculated were 40. Assuming a tray efficiency of 70%, this means that there are 55 total trays in the column. As defined in the presentation *Total Capital Investment and Cost Estimated – Distillation Column* given by Dr. Warren Seider on 11/19/2012, the calculations for the diameter, height, and cost of the distillation column are outlined below.
Estimating the Flooding Velocity:

$$U_f = C\left(\frac{\rho_L - \rho_G}{\rho_G}\right)$$

$$C = C_{SB} * F_{ST} * F_F * F_{HA}$$

For a non-foaming material, F_F =1, whereas F_{HA} must be determined for a sieve tray distillation column, dependent on the ratio of the active area of the distillation column to the total area of the tray. CSB is determined using Figure 19.4 in *Product and Process Design Principles*, whereas F_{ST} is defined as the following and is dependent on the surface tension of the mixture:

$$F_{ST} = \left(\frac{\sigma}{20}\right)^{0.2}$$

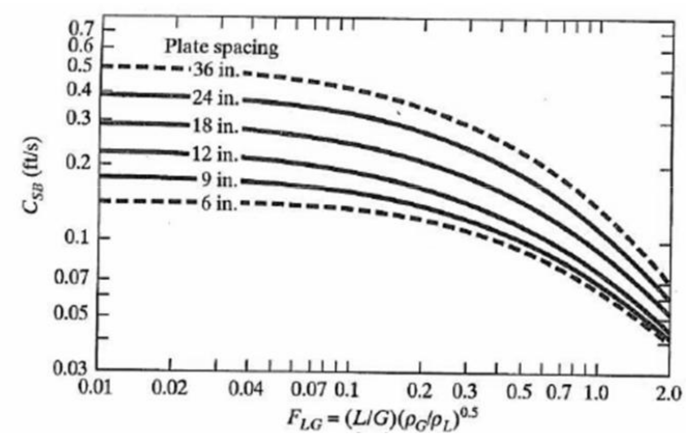
F_{ST} is calculated to be 0.9791 given the surface tension of the mixture at the top of the distillation tower is 18.1 lb/ft.
F_{LG} was also calculated using correlations from the ASPEN data. The density of the gas on the top tray is 0.11127 lb/ft3 while the density of the liquid fraction is 49.405 lb/ft3. Liquid flow rate is 365.316 lb/hr; vapor flow rate is 56.9179 lb/hr. These were put into the following equation to yield a F_{LG} of 0.3045.

$$F_{LG} = \left(\frac{L}{G}\right)\left(\frac{\rho_G}{\rho_L}\right)^{0.5}$$

To calculate the ratio, A_d/A_T, it may be estimated by the following:

$$\frac{A_d}{A_T} = 0.1 + \frac{F_{LG} - 0.1}{9}$$

This value turns out to be greater than 0.1, which means that the approximation where F_{HA} = 1 is the correct one, since for a sieve tray.
To calculate the last piece necessary to find the flooding velocity, the coefficient C_{SB} is determined from knowing 12 inch plate spacing along with the 0.3045 value of F_{LG}. Using the given graph below, C_{SB} is determined to be around 0.15.



Therefore, C for the flooding velocity equation is 0.146865. U_f, given these values, is around 2.63 ft/hr. Assuming that the actual velocity, U, is $0.85U_f$, the overall diameter of the tower can be calculated.

$$D = 2\left(\frac{V}{0.9\pi U}\right)^{0.5}$$

Where V is the vapor flow rate that was given by ASPEN earlier. Using this equation and the calculated variables, the overall estimated tower diameter is 5.5 ft, which can be increased to a standard size of 6ft.

With the diameter effectively calculated and the number of trays known (55 for this case with a spacing of 1 ft between each tray), the total tower cost can be determined. The total height, or length, is calculated by adding four feet for the top of the column with the condenser and ten feed at the bottom for the reboiler.

$$L = 54 * 1ft + 4ft + 10ft = 68ft$$

For the purchase and installed cost, the purchase cost of the column, not including the trays, is given by the equation below.

$$C_P = F_M C_V + C_{PL}$$

F_M is the materials factor, C_V is the vessel cost, and C_{PL} is the platform and ladder cost. To calculate the vessel cost, the weight of the tower must be estimated.

$$W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho$$

D and L are the inside diameter and length of the vessel as calculated previously. t_s is the thicknes of the material used, which in this case is carbon steel, meaning that the thickness can be assumed to be 0.75 inches. The density of the material, ρ, is 0.284 lb/in^2. Using this equation, the weight of the vessel is calculated as 42,500 lbs. C_V can then be calculated from the following equation.

$$C_V = \exp\left(7.2756 + 0.18255\ln(W) + 0.02297(\ln(W))^2\right)$$

From this, the vessel cost is $137,300 for 2006 with a CE of 500. To increase to 2013 costing, CE of 570 is used. The total cost for the vessel is then $156,500. Next the platform and ladder cost is evaluated.

$$C_{PL} = 300.9(D)^{0.63316}(L)^{0.80161}$$

This equation yields a cost for the ladders and platforms around $27,500. Again, to cost for 2013 a CE of 570 is used, making the cost of the ladders and platforms $31,400. Then the cost for the entire tower is calculated as follows. F_M is the materials factor which is 1 for carbon steel.

$$C_P = F_M C_V + C_{PL} = 1 * 156{,}500 + 31{,}400 = \$187{,}900$$

Next, the purchase cost of the trays needs to be calculated. Total cost of the trays, C_T, is calculated.

$$C_T = N_T F_{NT} F_{TT} F_{TM} C_{BT}$$

N_T is the total number of trays, F_{NT} is the number factor, which is 1 for towers with >20 trays. F_{TT} is the type factor, which is 1 for sieve trays; F_{TM} is the materials factor, equal to 1 for carbon steel. C_{BT} finally is the base cost for sieve trays, which is calculated with the equation below for 2006 values.

$$C_{BT} = 468e^{0.1739D}$$

Where D is again the diameter. C_{BT} is then $1,330 per tray.

$$C_T = N_T F_{NT} F_{TT} F_{TM} C_{BT} = 55 * 1 * 1 * 1 * \$1{,}330 = \$73{,}150$$

Therefore the total cost of the trays is $73,150 for 2006. Scaled to reflect 2013 prices, the cost is $83,400. The cost of the entire tower is then calculated with the equation below.

$$C_{BM} = F_{BM}(C_P + C_T) = 4.16(187{,}900 + 83{,}400) = \$1{,}128{,}600$$

F_{BM} is the bare module factor for a vertical pressure vessel. In this case, FBM is 4.16. Cost of the entire column is $1,128,600.

Reflux Accumulator:

For the reflux accumulator, this was sized and a cost estimated for it assuming that it is a horizontal pressure vessel. A typical aspect ratio, L/D for this type of a vessel is 2. The overall reflux ratio is 6.4183, with the reflux rate at 365.32 lb_{mol}/hr. Average molecular weight is 58.10 lb/ lb_{mol}. Density of this solution is assumed to be 50.23 lb/ft^3. The equation below outlines the total flowrate in ft^3/hr of the reflux.

$$Q = \frac{\left(365.32\frac{lb_{mol}}{\square r} * 58.10\frac{lb}{lb_{mol}}\right)}{50.23\frac{lb}{ft^3}} = \frac{422.55 ft^3}{\square r}$$

With a typical residence time of 5 minutes (assuming the vessel is actually only half full for this particular residence time), the total diameter of the reflux accumulator can be determined. The total volume of the container, then, would be

$$V = 2Q\tau$$

As outlined in the equation below, the diameter is dependent on the residence time and the volumetric flow rate of the liquid going into the reflux accumulator. Assuming the vessel is a cylinder in shape, the diameter of the vessel would be:

$$D = \left(\frac{4Q\tau}{\pi}\right)^{0.33}$$

Using the flow rate and residence time specified above, the diameter is calculated to 3.55 ft. Then the total length of the vessel is twice that amount, or 7.1 ft.

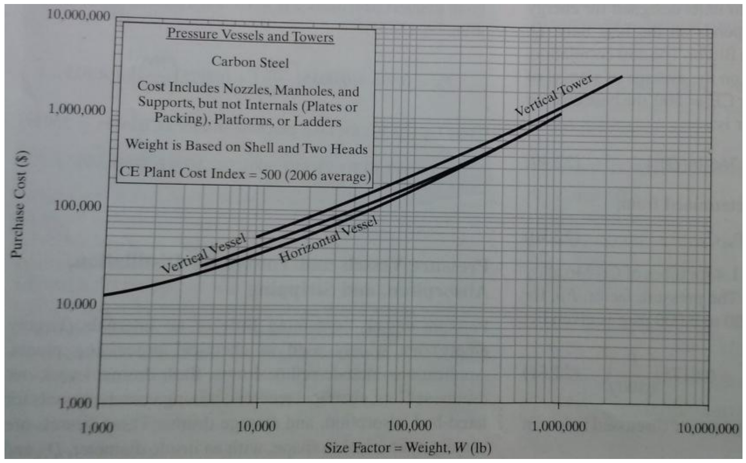
From here, the correlations based on f.o.b. purchase costs for pressure vessels and towers can be used to calculate the cost of the reflux accumulator. To find the overall cost, the weight of the shell with the two heads is approximated by the same weighting equation as seen for the tower.

$$W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho$$

With the diameter calculated at Xft and the length at Xft, the overall weight is calculated to be XX,XXX lbs. Using the correlations for carbon steel in Seider's text, pg 574, the following graph can correctly calculated the horizontal tower's (reflux accumulator's) total cost. Thickness of the vessel is again 0.75 inches with the density of carbon steel at 0.284 lb/in^2.

$$W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho$$

$$= \pi(3.55 * 12 + 0.75)(7.1 * 12 + 0.8 * 3.55 * 12)0.75 * 0.284 = 3{,}460 \text{ lbs}$$



The total cost of the reflux accumulator, given by the graph, is around $20,000 for 2006. Scaled to fit 2013 costing, the total cost comes to around $22,800. However, the bare modulus factor of 4.16 must also be multiplied to get the final cost of this horizontal tower. Multiplying the cost by 4.16 gives a final cost estimate at $94,800.

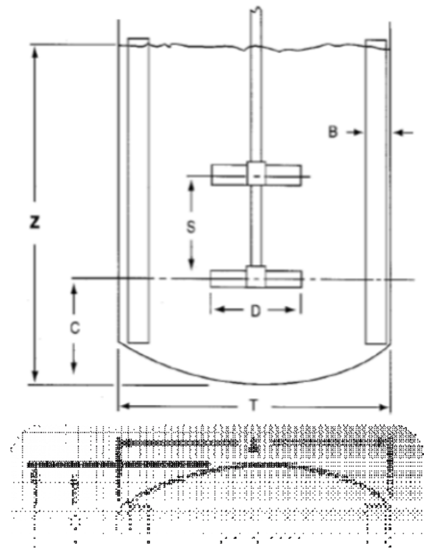
Condenser/Reboilder:
Modeled as heat exchangers. See Heat Exchangers sample calculations.

Reflux Pump:
Modeled as pump. See Pump sample calculations.

Sample Agitator Calculations for R-202

The entire sizing for the agitators were performed using the following spreadsheet entitled "Agitator Power Requirement and Mixing Intensity Calculations" obtained from cheresources.com. By inputting the reactor geometry, selecting the type of agitator, inputting the fluid properties in the vessel, the power requirement required for the correlations in *Seider et al.* (SSLW 22.23) would be calculated.

Reactor Geometry					
Diameter of the reactor	T	=	13.63940513	ft	
Height of the cylindrical portion	H	=	47.7	ft	
Liquid level height in the reactor from bottom	Z	=	32.95460831	ft	
Total Volume of the reactor	V	=	204.6	m3	
Select the type of Agitator			Pitched Blade Turbine		
D/T Ratio			0.5		
Agitator rpm	N	=	110	rpm	
Fluid Properties					
Density	ρ	=	63.69798	kg/m3	
Viscosity	μ	=	100	cp	
Calculation					
1) Reynolds Number					
Diameter of the agitator	D	=	2.1	m	
Reynolds Number	Re	=	5046		
2)Power Requirement					
Power Number	Np	=	1.37		Select the value from Power number chart based on Reynolds number
Power Required (Assuming 80% Loading)	P	=	34.98	hp	Use 5.5 for Rushton six blade turbine & 3.2 for concave 180 degree turbine
3) Mixing Intensity					
Pumping Number	Nq	=	0.6		Select the value from Pumping number chart based on Reynolds number
Equivalent Diameter	Teq	=	20.95	ft	Use 0.72 for Rushton six blade turbine & 0.7 for concave 180 degree turbine
Volumetric flow rate	Q	=	348.6	ft3/sec	
Cross sectional area	A	=	146.0	ft2	
Velocity	V	=	2.387	ft/sec	Click here
4) Agitator required					
No of Agitators Required		=	2		Click Here



Also, the following are correlations from Seider for which a turbine agitator in a closed vessel would be cost.

Agitator (Turbine, closed vessel)

Applicable Blocks: R-202A, R-202B, R-202C, N-301

Variable	Description	Unit
S	Size Factor = Motor Hp	hp

Relevant Equations: **Source**

1) Find Equipment Cost

C_B	=	$3620 \times S^{0.57}$	Includes speed reducer, pressures to 150 psig	SSLW (22.23)

5) Find Total Vertical Pressure Vessel Cost

F_M	=	1	SSLW (pg580)
C_P	=	$C_B \times F_M$	
C_P (CE=575.	=	$(575.4/500)*C_p$	

Sample Blower Calculations (B-101)

From ASPEN, the brake horsepower, P_B (hp) of B-101 is 2.3 hp.

The fractional efficiency of the electric motor is calculated using (SSLW 22.18) :

$$\eta_M = 0.80 + 0.0319(\ln P_B) - 0.00182(\ln P_B)^2; \text{For } 1 < P_B < 1500\ Hp$$

$$\eta_M = 0.80 + 0.0319(\ln 2.3\text{ Hp}) - 0.00182(\ln 2.3)^2 = 0.83$$

The power consumption, P_C (hp):

$$P_C = \frac{P_B}{\eta_M} = \frac{2.3\text{ hp}}{0.83} = 2.8\text{ hp}$$

Cost

For a cast iron (F_M = 1) centrifugal blower, the f.o.b. purchase cost, CE Index = 500, is given by (from SSLW (T22.32))

$$C_{FOB} = e^{6.8929+0.7900(\ln P_C)} = e^{6.8929+0.7900(\ln 2.8\text{ hp})} = \$\ 2{,}220$$

The bare-module factor, F_{BM} gas compressors and drivers = 2.15 (SSLW T22.11)

Therefore, the equipment bare-module cost, CE Index = 575.4 is:

$$C_P = \left(\frac{CE_{575.4}}{CE_{500}}\right) \times C_{FOB} \times F_{BM} = \left(\frac{575.4}{500}\right) \times (\$\ 2{,}220) \times (2.15) = \$\ 5{,}490$$

Centrifugal Blower
Applicable Blocks: B-201, B-202, B-203

Variable	Description	Unit
Q	Inlet Volumetric Flow Rate	ft^3/min
P_i	Inlet Pressure	psi
P_o	Outlet Pressure	psi

Relevant Equations: **Source**

1) Find Consumed Power

η_B	=	0.75		
P_B	=	$0.00436\times(k/(k-1))\times(Q\times P_i/\eta_B)\times((P_o/P_i)^{(k-1)/k}-1)$	Brake horsepower	SSLW (22.30)
η_M	=	$0.80+0.0319\times \ln(P_B)-0.00182\times\ln(P_B)^2$	Motor efficiency	SSLW (22.18)
P_C	=	P_B / η_M	Size factor	

2) Find Total Blower Cost

C_B	=	$\exp(6.8929+0.7900\times \ln(P_C))$	SSLW (22.32)
F_M	=	1 (Cast Iron)	
C_{FOB}	=	$C_B \times F_M$	SSLW (T22.11)
F_{BM}	=	2.15	
C_P	=	$C_{FOB} \times F_{BM}$	

Sample Compressor Calculations (C-101)

From ASPEN, the brake horsepower, P_B (hp) of C-101 is 22.3 hp.

The fractional efficiency of the electric motor is calculated using (SSLW 22.18) :

$$\eta_M = 0.80 + 0.0319(\ln P_B) - 0.00182(\ln P_B)^2; \text{ For } 1 < P_B < 1500\ Hp$$

$$\eta_M = 0.80 + 0.0319(\ln 22.3 \text{ Hp}) - 0.00182(\ln 22.3)^2 = 0.88$$

The power consumption, P_C (hp):

$$P_C = \frac{P_B}{\eta_M} = \frac{22.3 \text{ hp}}{0.88} = 25.3 \text{ hp}$$

Cost

For a cast iron ($F_M = 1$) screw compressor (valid from $10 < P_C < 750$ hp), the f.o.b. purchase cost, CE Index = 500, is given by (from SSLW (22.38))

$$C_{FOB} = e^{8.1238+0.7243(\ln P_C)} = e^{8.1238+0.7243(\ln 2.8 \text{ hp})} = \$\,35{,}050$$

The bare-module factor, F_{BM} gas compressors and drivers = 2.15 (SSLW T22.11). Therefore, the equipment bare-module cost, CE Index = 575.4 is:

$$C_P = \left(\frac{CE_{575.4}}{CE_{500}}\right) \times C_{FOB} \times F_{BM} = \left(\frac{575.4}{500}\right) \times (\$\,35{,}050) \times (2.15) = \$\,86{,}800$$

Centrifugal Compressor
Applicable Blocks: C-101, C-102, C-103, C-301

Variable	Description	Unit
Q	Volumetric Flow Rate	gal/min
P_i	Inlet Pressure	psi
P_o	Outlet Pressure	psi

Relevant Equations:			**Source**
1) Find Consumed Power			
η_B	=	0.75	
P_B	=	$0.00436\times(k/(k-1))\times(Q\times P_i/\eta_B)\times((P_o/P_i)^{(k-1)/k}-1)$	SSLW (22.30)
η_M	=	$0.80+0.0319\times ln\,(P_B)-0.00182\times \ln(P_B)^2$	SSLW (22.18)
P_C	=	P_B / η_M	
2) Find Total Blower Cost			
C_B	=	$exp\,(6.8929+0.7900\times ln\,(P_C))$	SSLW (22.32)
F_M	=	1 (Cast Iron)	
C_{FOB}	=	$C_B \times F_M$	SSLW (T22.11)
F_{BM}	=	2.15	
C_P	=	$C_{FOB} \times F_{BM}$	

Sample Vapor Liquid Separator Calculations

All the sizing and costing for the vapor liquid separators/flash vessels were performed using ASPEN Process Economic Analyzer (IPE). The following are correlations from *Product and Process Design Principles* for which a flash vessel would be sized and cost. Equivalently, the spreadsheet provided by Mr. Fabiano was also used to size the flash vessel as a comparison.

Vapor Liquid Separator

Applicable Blocks: F-201, F-301

Variable	Description	Unit	
Q	Volumetric Flow Rate	ft^3/min	
τ	Residence Time	min	
AR	Aspect Ratio, AR = L/D	*dimensionless*	
P_o	Operating Pressure	psig	
E	Weld Efficiency	*dimensionless*	= 0.85 for thickness < 1.25 in.
S	Maximum Allowable Shell Stress	psi	
ρ_S	Density of Carbon Steel	lb/in^3	

Relevant Equations: **Source**

1) Find Volume

Holdup	=	$Q \times \tau$	ft^3	
V	=	$2 \times \text{Holdup}$	ft^3	

2) Find Diameter and Length

D	=	$((2\times V)/\pi)^{1/3}$	ft	
L	=	$D \times AR$	ft	

3) Shell Thickness, excl. wind and earthquake considerations

			Source
P_d	=	$exp\,(0.60608 + 0.91615\times ln\,(P_o) + 0.0015655\times ln\,(P_o)^2$	SSLW (22.61)
t_p	=	$(P_d \times D) / (2 \times S \times E - 1.2 \times P_d)$	SSLW (22.60)
t_C	=	0.125 (in) Corrosion Allowance	
t_S	=	$t_p + t_c$	

4) Find Vessel Weight and Cost

			Source
W	=	$\pi \times (D + t_s) \times (L + 0.8 \times D) \times t_V \times \rho_S$	SSLW (22.59)
C_V	=	$exp\,(7.2756 + 0.18255\times ln\,(W) + 0.02297\times ln\,(W)^2$	SSLW (22.53)
F_M	=	1 Carbon Steel	
C_{VESSEL}	=	$C_V \times F_M$	

5) Find Cost of Platforms and Ladders

			Source
C_{PL}	=	$300.9\times D^{0.63316}\times L^{0.80161}$	SSLW (22.58)

6) Find Total Vertical Pressure Vessel Cost

			Source
C_{FOB}	=	$C_{VESSEL} \times C_{PL}$	
F_{BM}	=	4.16	SSLW (T22.11)
C_P	=	$C_{FOB} \times F_{BM}$	

Sample Heat Exchanger Calculations

All the sizing for the heat exchangers was performed using ASPEN Plus Exchanger Design and Rating (EDR) and costing was done using ASPEN Process Economic Analyzer (IPE). The following are correlations from *Product and Process Design Principles* for which a shell-and-tube heat exchanger would be sized and cost.

Shell and Tube Heat Exchanger (Fixed Head)
Applicable Blocks:

Variable	Description	Unit
$T_{h,in}$	Initial temperature of the hot stream	°F
$T_{h,out}$	Final temperature of the hot stream	°F
$T_{c,in}$	Initial temperature of the cold stream	°F
$T_{c,out}$	Final temperature of the cold stream	°F
Q	Heat duty	Btu
U	Overall heat exchange coefficient	Btu/ft^2-hr-°F
L	Tube length	ft
P_S	Shell pressure	psig
a	Material of construction factor	*dimensionless*
b	Material of construction factor	*dimensionless*

Relevant Equations: **Source**

1) Find the Log-Mean Temperature Difference

			Source
ΔT_1	=	$T_{h,in} - T_{c,out}$	SSLW (S18.3)
ΔT_2	=	$T_{h,out} - T_{c,in}$	SSLW (S18.3)
ΔT_{LM}	=	$(\Delta T_1 - \Delta T_2) / \ln((\Delta T_1 / \Delta T_2)$	SSLW (18.3)

2) Find the Area Required for Heat Exchange

			Source
A	=	$Q / (U \times \Delta T_{LM})$	SSLW (S18.3)

3) Find Vessel Cost

			Source
F_M	=	$a + (A/100)^b$	SSLW (22.44)
F_L	=	1 L = 20 ft	SSLW (S22.5)
F_P	=	$0.9803 + 0.018(P_S/100) + 0.0017(P_S/100)^2$	SSLW (22.45)
C_B	=	$\exp(11.0545 - 0.9228 \times \ln(A) + 0.09861 \times \ln(A)^2$	SSLW (22.40)
C_{FOB}	=	$F_M \times F_L \times F_P \times C_B$	
F_{BM}	=	3.17	
C_P	=	$C_{FOB} \times F_{BM}$	SSLW (T22.11)

Sample Vertical Pressure Vessel Calculations

The following are correlations from *Product and Process Design Principles* for which a vertical pressure vessel would be sized and cost.

Vertical Pressure Vessel

Applicable Blocks: R-202A, R-202B, R-202C, DC-301, N-301

Variable	Description	Unit
Q	Volumetric Flow Rate	ft^3/min
τ	Residence Time	min
AR	Aspect Ratio	*dimensionless*
P_o	Operating Pressure	psig
E	Weld Efficiency	*dimensionless*
S	Maximum Allowable Shell Stress	psi
ρ_S	Density of Carbon Steel	lb/in^3

Relevant Equations: **Source**

1) Find Diameter and Length

V	=	$Q \times \tau$	
D	=	$((4 \times V) / (AR \times \pi))^{1/3}$	
L	=	$D \times AR$	

2) Shell Thickness

P_d	=	$exp\,(0.60608 + 0.91615 \times ln\,(P_o) + 0.0015655 \times ln\,(P_o)^2$	SSLW (22.61)
t_p	=	$(P_d \times D) / (2 \times S \times E - 1.2 \times P_d)$	SSLW (22.60)
t_C	=	0.125 (in) Corrosion Allowance	
t_S	=	$t_p + t_c$	

3) Find Vessel Weight and Cost

W	=	$\pi \times (D + t_s) \times (L + 0.8 \times D) \times t_V \times \rho_S$	SSLW (22.59)
C_V	=	$exp\,(7.2756 + 0.18255 \times ln\,(W) + 0.02297 \times ln\,(W)^2$	SSLW (22.53)
F_M	=	1 Carbon Steel	
C_{VESSEL}	=	$C_V \times F_M$	

4) Find Cost of Platforms and Ladders

C_{PL}	=	$300.9 \times D^{0.63316} \times L^{0.80161}$	SSLW (22.58)

5) Find Total Vertical Pressure Vessel Cost

C_{FOB}	=	$C_{VESSEL} \times C_{PL}$	
F_{BM}	=	4.16	SSLW (T22.11)
C_P	=	$C_{FOB} \times F_{BM}$	

Sample Pump Calculations

All the sizing for the pumps performed using ASPEN Process Economic Analyzer (IPE). The following are correlations from *Product and Process Design Principles* for which a pump would be sized and cost as a comparison.

Centrifugal Pump
Applicable Blocks: P-101, P-102, P-103, P-201, P-202, P-203, P-204, P-301

Variable	Description	Unit
Q	Volumetric Flow Rate	gal/min
ΔP	Pressure Rise	psi
ρ_L	Liquid Density	lb/gal
A_G	Gravitational Acceleration	ft/s^2

Relevant Equations: **Source**

1) Find Pump head

P_H	=	$(\Delta P \times 144)/(\rho_L \times A_G)$	ft

2) Find Pump Cost

			Source
S	=	$Q \times P_H^{0.5}$	SSLW (22.13)
C_B	=	$exp\,(9.7171 - 0.6019 \times ln\,(S) + 0.0519 \times ln\,(S)^2)$	SSLW (22.14)
F_M	=	1 (Cast Iron)	SSLW (S22.5)
F_T	=	1.0 $50 < P_H < 400$, $hp_{max} = 75$	SSLW (S22.5)
		1.5 $50 < P_H < 200$, $hp_{max} = 200$	
		1.7 $100 < P_H < 450$, $hp_{max} = 150$	
		2.0 $50 < P_H < 500$, $hp_{max} = 250$	
		2.7 $300 < P_H < 1{,}100$, $hp_{max} = 250$	
		8.9 $650 < P_H < 3{,}200$, $hp_{max} = 1{,}450$	
C_{PUMP}	=	$C_B \times F_M \times F_T$	

3) Find Motor Cost

			Source
η_P	=	0.7	
P_B	=	$(Q \times P_H \times \rho_L)/(33{,}000 \times \eta_P)$	SSLW (22.16)
η_M	=	$0.80 + 0.0319 \times ln\,(P_B) - 0.00182 \times \ln(P_B)^2$	SSLW (22.18)
P_C	=	$(Q \times P_H \times \rho_L)/(33{,}000 \times \eta_P \times \eta_M)$	SSLW (22.16)
C_B	=	$exp\,(5.8259 + 0.13141 \times ln\,(P_C) + 0.053255 \times ln\,(P_C)^2 + 0.028628 \times ln\,(P_C)^3 - 0.0035549 \times ln\,(P_C)^4)$	SSLW (22.19)
F_T	=	1.8 Explosion-proof Enclosure	SSLW (S22.5)
C_{MOTOR}	=	$C_B \times F_T$	

4) Find Total Cost

			Source
C_{FOB}	=	$C_B \times F_T$	SSLW (T22.11)
F_{BM}	=	3.3	
C_P	=	$C_{FOB} \times F_{BM}$	

Sample Reactor Calculations (R-202A, B, C)

The following calculations serve as a supplement to the methodology outlined in the 'B. ii. Reactor Design' section of the paper. A lot of the reasoning behind these calculations can be found with reference to the afore-mentioned section. The calculations are broken down into several steps that correspond with the 'Reactor Design' subsections for easy reading.

Vessel Sizing

The volumetric flow rate, Q of the stream (S-206) entering R-202A is $1457\ \mathrm{ft^3/hr}$ (from ASPEN)

The appropriate residence time, τ of the whole cascade is 12 hours as determined from literature references to give the maximum niacinamide concentration; hence, the residence time, τ for each vessel is 4 hours.

Total Volume of vessel, $\mathrm{V = Q \times \tau = 1457\ \frac{ft^3}{hr} \times 4\ hr = 5830\ ft^3}$

From ASPEN, the vapor fraction obtained is 0.463 giving the volume of vapor and liquid as:

$\mathrm{V_{vapor} = 0.463 \times V = 2700\ ft^3}$

$\mathrm{V_{liquid} = (1 - 0.463) \times V = 3130\ ft^3}$

Adjusting the volume for liquid in the vapor phase:

$\mathrm{V_{vapor,adj.} = 0.8 \times V_{vapor} = 2160\ ft^3}$

Adjusting the volume for vapor dissolved in the liquid phase:

$\mathrm{V_{liquid,adj.} = \frac{V_{liquid}}{0.65} = 4815\ ft^3}$

Total adjusted volume, $\mathrm{V_{total,adj.} = V_{vapor,adj.} + V_{liquid,adj.} = 6975\ ft^3}$

Selecting an aspect ratio, AR = L/D as 3.5. The diameter, D and height, L of the vessel was determined to be 14 ft and 48 ft respectively.

Vessel Costing

Correlations from SSLW were used. Please refer to Sample Vertical Pressure Vessel Calculations on page 245.

Agitator Sizing and Costing

Please refer to Sample Agitator Calculations for R-202 on page 239. The number of impellers required and their individual power requirements were determined for costing using correlations in *Product and Process Design Principles*.

Sample Storage Vessel Calculations (T-101)

From ASPEN, the outlet volumetric flow rate, Q_o (gal/hr) of T-101 (S-101) is 404 gal/hr. With a residence time, τ (hr) of 7 days or 168 hours and maintaining it at 60% (f = 0.6) of the tank capacity for potential increase in productions, the tank volume, V (gal):

$$V = \frac{Q_o \times \tau}{f} = \frac{(404\ \frac{gal}{hr}) \times (168\ hr)}{0.6} = 113{,}000\ gal$$

Cost

For a cast iron ($F_M = 1$) floating roof storage tank, the f.o.b. purchase cost, CE Index = 500, is given by (from SSLW (T22.32))

$$C_{FOB} = 475 \times V^{0.51} = 475 \times (113{,}000\ gal)^{0.51} = \$\ 179{,}400$$

The bare-module factor, F_{BM} for horizontal pressure vessels = 3.05 (SSLW T22.11)

Therefore, the equipment bare-module cost, CE Index = 575.4 is:

$$C_P = \left(\frac{CE_{575.4}}{CE_{500}}\right) \times C_{FOB} \times F_{BM} = \left(\frac{575.4}{500}\right) \times (\$\ 179{,}400) \times (3.05) = \$\ 629{,}600$$

Floating Roof Storage Tank

Applicable Blocks: T-101

Variable	Description	Unit
Q	Inlet/Outlet Volumetric Flow Rate	gal/hr
τ	Residence Time	hr

Relevant Equations: **Source**

1) Find the Tank Volume

$V = Q \times \tau$

2) Calculate Vessel Cost

			Source
C_{FOB}	=	$475 \times V^{0.51}$	SSLW (T22.32)
F_{BM}	=	3.05	SSLW (T22.11)
C_P	=	$C_{FOB} \times F_{BM}$	

Cone-Roof Storage Tank

Applicable Blocks: T-301

Variable	Description	Unit
Q	Inlet/Outlet Volumetric Flow Rate	gal/hr
τ	Residence Time	hr

Relevant Equations: **Source**

1) Find the Tank Volume

$V = Q \times \tau$

2) Calculate Vessel Cost

			Source
C_{FOB}	=	$265 \times V^{0.51}$	SSLW (T22.32)
F_{BM}	=	4.16	SSLW (T22.11)
C_P	=	$C_{FOB} \times F_{BM}$	

E. PROFITABILITY ANALYSIS SPREADSHEET

Process Title:	***Green Process to Produce Niacin***	
Product:	***Niacinamide***	
Plant Site Location:	***Michigan***	
Timeline:		
Number of Years for Design	1	(must be whole number)
Number of Years for Construction	1	(must be whole number)
Number of Years for Production	18	
Total Number of Years for Project	20	
Start Year	2013	
Site Factor	1.00	
Continuous Operation:		
Days per Year	0	
OR		
Hours per Year	8026	
OR		
Operating Factor	0.0000	(if multiple entries, "Operating Factor" is used)
Discrete Operation:		(cannot use Continuous AND Discrete. If both entered, Discrete used by default)
Hours per Day	0	
AND		
Days per Year	0	
Production Capacity	90%	of Design Capacity
Start production at	50%	of Production Capacity
Years to achieve full capacity	2	
Number of Shifts	5	
Depreciation Schedule	5 year	
Income Tax Rate	37%	
Cost of Capital (for the NPV Calculation)	15%	(discount rate)
General Inflation Rate	2%	
Product Inflation Rate	0%	
Variable Cost Inflation Rate	0%	
Fixed Cost Inflation Rate	0%	
Product Information:		
Enter Product Units	*lb*	
(i.e. lb, gram, gal, etc)		
Price Per Unit	$4.43	/lb
Number of units per:	(Specify ONE of the three. If multiple entries, "Year" is used.)	
Year	27,701,739	lb per Year
OR		
Day	-	lb per Day
OR		
Hour	-	lb per Hour

Raw Materials						
	Raw Material:	**Unit:**	**Required Ratio:**		**Cost of Raw Material:**	
1	MPDA	lb	0.958090595	lb per lb of Niacinamide	$3.091	per lb
2	Nitrogen	MT	4.06E-12	MT per lb of Niacinamide	$110.000	per MT
3	Oxygen	MT	1.94E-10	MT per lb of Niacinamide	$77.000	per MT
4	Process Water	lb	0.34766606	lb per lb of Niacinamide	$7.500E-04	per lb
5						
6						
7						
8						
9						
10						
	Total Weighted Average:				$2.962	per lb of Niacinamide
Byproducts						
	Byproduct:	**Unit:**	**Ratio to Product**		**Byproduct Selling Price**	
1						
2						
3						
4						
5						
6						
7						
8						
9						
10						
	Total Weighted Average:				$0.000E+00	per lb of Niacinamide
Utilities						
	Utility:	**Unit:**	**Required Ratio**		**Utility Cost**	
1	High Pressure Steam	lb	9.0943	lb per lb of Niacinamide	$7.520E-03	per lb
2	Critical Refrigeration	ton-day	0.001212	ton-day per lb of Niacinamide	$3.990	per ton-day
3	Refrigeration	ton-day	0.0067607	ton-day per lb of Niacinamide	$2.440	per ton-day
4	Cooling Water	lb	489.399	lb per lb of Niacinamide	$8.550E-05	per lb
5	Electricity	kWh	4.98E-01	kWh per lb of Niacinamide	$0.068	per kWh
6	Hot Water	lb	0.3494043	lb per lb of Niacinamide	$8.550E-04	per lb
7						
8						
9						
10						
	Total Weighted Average:				$0.166	per lb of Niacinamide

	MACRS Depreciation Schedule:				
	5 year	***7 year***	***10 year***	***15 year***	***20 year***
1	20.00%	14.29%	10.00%	5.00%	3.75%
2	32.00%	24.49%	18.00%	9.50%	7.22%
3	19.20%	17.49%	14.40%	8.55%	6.68%
4	11.52%	12.49%	11.52%	7.70%	6.18%
5	11.52%	8.93%	9.22%	6.93%	5.71%
6	5.76%	8.92%	7.37%	6.23%	5.29%
7		8.93%	6.55%	5.90%	4.89%
8		4.46%	6.55%	5.90%	4.52%
9			6.56%	5.91%	4.46%
10			6.55%	5.90%	4.46%
11			3.28%	5.91%	4.46%
12				5.90%	4.46%
13				5.91%	4.46%
14				5.90%	4.46%
15				5.91%	4.46%
16				2.95%	4.46%
17					4.46%
18					4.46%
19					4.46%
20					4.46%
21					2.23%

Other Variable Costs

General Expenses

Selling / Transfer Expenses:	3.00%	of Sales
Direct Research:	4.80%	of Sales
Allocated Research:	0.50%	of Sales
Administrative Expense:	2.00%	of Sales
Management Incentive Compensation:	1.25%	of Sales

Working Capital

Accounts Receivable	⇨	**30**	**Days**
Cash Reserves (excluding Raw Materials)	⇨	**30**	**Days**
Accounts Payable	⇨	**30**	**Days**
Niacinamide Inventory	⇨	**2**	**Days**
Raw Materials	⇨	**7**	**Days**

	% of Total Permanent Investment					
2014	100%		(default is first year of Construction, otherwise over-ride this year)			
2015	0%					
2016	0%					
2017	0%					
	Cost of Site Preparations:		5.00%	of Total Bare Module Costs		
	Cost of Service Facilities:		5.00%	of Total Bare Module Costs		
Allocated Costs for utility plants and related facilities:			$500,000			
Cost of Contingencies and Contractor Fees:			18.00%	of Direct Permanent Investment		
		Cost of Land:	2.00%	of Total Depreciable Capital		
		Cost of Royalties:	2.00%			
		Cost of Plant Start-Up:	10.00%	of Total Depreciable Capital		

Equipment Costs

Equipment Description	Type	Purchase Cost	Bare Module Factor	Bare Module Cost
Name	(must be filled-in!)		(default 3.21 if blank)	
A-101	Fabricated Equipment	791,116	4	$3,291,044
A-102	Fabricated Equipment	548,989	4	$2,283,795
B-201	Process Machinery	2,555	2	$5,492
B-202	Process Machinery	2,304	2	$4,954
B-203	Process Machinery	2,828	2	$6,080
C-101	Process Machinery	40,335	2	$86,719
C-102	Process Machinery	94,138	2	$202,397
C-103	Process Machinery	118,025	2	$253,753
C-301	Process Machinery	1,084,345	2	$2,331,342
D-101	Fabricated Equipment	967,255	4	$4,023,779
DC-301	Fabricated Equipment	38,089	4	$149,787
DR-301	Fabricated Equipment	804,369	2	$1,657,000
F-201	Fabricated Equipment	128,760	4	$535,640
F-301	Fabricated Equipment	115,273	4	$479,535
HX-101	Fabricated Equipment	76,656	3	$243,001
HX-102	Fabricated Equipment	74,697	3	$236,789
HX-201	Fabricated Equipment	133,947	3	$424,612
HX-202A	Fabricated Equipment	104,322	3	$330,700
HX-202B	Fabricated Equipment	77,117	3	$244,462
HX-203	Fabricated Equipment	57,636	3	$182,707
HX-204	Fabricated Equipment	57,636	3	$182,707
HX-205	Fabricated Equipment	72,622	3	$230,211
HX-206	Fabricated Equipment	53,371	3	$169,187
HX-301	Fabricated Equipment	66,282	3	$210,113
HX-302	Fabricated Equipment	123,457	3	$391,359
HX-303	Fabricated Equipment	56,829	3	$180,149
HX-304A	Fabricated Equipment	253,139	3	$802,450
HX-304B	Fabricated Equipment	88,414	3	$280,273
N-301	Fabricated Equipment	45,900	4.16	142,736
P-101	Process Machinery	30,547	3	$100,806
P-102	Process Machinery	30,432	3	$100,426
P-103	Process Machinery	41,844	3	$138,085
P-201	Process Machinery	34,467	3	$113,740
P-202	Process Machinery	34,467	3	$113,740
P-203	Process Machinery	34,467	3	$113,740
P-204	Process Machinery	31,239	3	$103,088
P-301	Process Machinery	36,541	3	$120,587
R-101	Other Equipment	810,184	3	$2,568,283
Additional Equipment				$10,733,767
Total				***33,769,035***

(Note: The first 38 equipment items are displayed in the Input Summary tab. Items listed below are included in calculating the total bare module cost.)

ADDITIONAL EQUIPMENT				
Equipment Description		**Purchase Cost**	**Bare Module Factor**	**Bare Module Cost**
Name	**Type**		(default 3.21 if blank)	
R-102	Other Equipment	$30,713	3	$97,359
R-201	Other Equipment	$721,219	3	$2,286,265
R-202A	Other Equipment	$268,719	3	$918,160
R-202B	Other Equipment	$268,719	3	$918,160
R-202C	Other Equipment	$268,719	3	$918,160
T-101	Storage	$206,429	3	$629,609
T-301	Storage	$104,337	4	$434,044
Wastewater Treatment	Other Equipment			$239,065
Wastegas Treatment	Other Equipment			$40,000
Wastegas Treatment	Other Equipment			$40,000
Dowtherm System	Other Equipment			$722,207
Reactor 1 Catalyst	Catalysts	$3,808	1	$3,808
Reactor 2 Catalyst	Catalysts	$783,300	1	$783,300
Reactor 3	Catalysts	$1,645,510	1	$1,645,510
Reactor 4	Catalysts	$153,910	1	$153,910
P-101	Spares	30,547	3	$100,806
P-102	Spares	30,432	3	$100,426
P-103	Spares	41,844	3	$138,085
P-201	Spares	34,467	3	$113,740
P-202	Spares	34,467	3	$113,740
P-203	Spares	34,467	3	$113,740
P-204	Spares	31,239	3	$103,088
P-301	Spares	36,541	3	$120,587

Bare Module Factor Calculator:

Use the tool below to calculate a particular bare module factor, then input in the required column to the left:

(Note, if no bare module factor is entered, the default of 3.21 will be used)

Cost of Installation Materials:	**71%**	of Equipment Purchase Cost
Cost of Installation Labor:	**54%**	of Equipment Purchase Cost
Cost for Freight, Insurances, and Taxes:	**9%**	of Equipment Purchase Cost
Cost of Construction Overhead:	**57%**	of Equipment Purchase Cost
Cost of Contractor Engineering Expenses:	**30%**	of Equipment Purchase Cost
Total Derived Bare Module Factor:	***3.21***	of Equipment Purchase Cost

Fixed Costs					
	Operations				
	Operators per Shift:	1	(assuming	5	shifts)
	Direct Wages and Benefits:	$35	/operator hour		
	Direct Salaries and Benefits:	15%	of Direct Wages and Benefits		
	Operating Supplies and Services:	6%	of Direct Wages and Benefits		
	Technical Assistance to Manufacturing:	$0.00	per year, for each Operator per Shift		
	Control Laboratory:	$0.00	per year, for each Operator per Shift		
	Maintenance				
	Wages and Benefits:	4.50%	of Total Depreciable Capital		
	Salaries and Benefits:	25.00%	of Maintenance Wages and Benefits		
	Materials and Services:	100.00%	of Maintenance Wages and Benefits		
	Maintenance Overhead:	5.00%	of Maintenance Wages and Benefits		
	Operating Overhead				
	General Plant Overhead:	7.10%	of Maintenance and Operations Wages and Benefits		
	Mechanical Department Services:	2.40%	of Maintenance and Operations Wages and Benefits		
	Employee Relations Department	5.90%	of Maintenance and Operations Wages and Benefits		
	Business Services	7.40%	of Maintenance and Operations Wages and Benefits		
	Property Taxes and Insurance				
	Property Taxes and Insurance:	2.00%	of Total Depreciable Capital		
	Straight Line Depreciation				
	Direct Plant:	8.00%	of Total Depreciable Capital, less	1.18	times the Allocated Costs for Utility Plants and Related Facilities
	Allocated Plant:	6.00%	of	1.18	times the Allocated Costs for Utility Plants and Related Facilities
	Other Annual Expenses				
	Rental Fees (Office and Laboratory Space):	$0			
	Licensing Fees:	$0			
	Miscellaneous:	$0			
	Depletion Allowance				
	Annual Depletion Allowance:	$0			

F. MSDS and Compound Data

Reactivity Hazard: 0

Potential Health Effects

Inhalation	May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Skin	May be harmful if absorbed through skin. Causes skin burns.
Eyes	Causes eye burns.
Ingestion	May be harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Formula : C6H16N2
Molecular Weight : 116.20 g/mol

Component		Concentration
2-Methylpentane-1,5-diamine		
CAS-No.	15520-10-2	-
EC-No.	239-556-6	

4. FIRST AID MEASURES

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

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

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

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

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Suitable extinguishing media
For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx)

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Fluka - 33120 Page 2 of 7

SIGMA-ALDRICH sigma-aldrich.com

Material Safety Data Sheet
Version 3.2
Revision Date 09/21/2012
Print Date 01/13/2013

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	: 2-Methylpentane-1,5-diamine
Product Number	: 33120
Brand	: Fluka
Supplier	: Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	: +1 800-325-5832
Fax	: +1 800-325-5052
Emergency Phone # (For both supplier and manufacturer)	: (314) 776-6555
Preparation Information	: Sigma-Aldrich Corporation Product Safety - Americas Region 1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Combustible Liquid, Harmful by ingestion., Corrosive

GHS Classification
Flammable liquids (Category 4)
Acute toxicity, Oral (Category 4)
Skin corrosion (Category 1B)
Serious eye damage (Category 1)

GHS Label elements, including precautionary statements

Pictogram 

Signal word Danger

Hazard statement(s)

H227	Combustible liquid
H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.

Precautionary statement(s)

P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER or doctor/ physician.

HMIS Classification

Health hazard:	3
Flammability:	2
Physical hazards:	0

NFPA Rating

Health hazard:	3
Fire:	2

Fluka - 33120 Page 1 of 7

Upper explosion limit	no data available
Vapour pressure	173 hPa (130 mmHg) at 135 °C (275 °F)
Density	0.865 g/cm3
Water solubility	no data available
Partition coefficient: n-octanol/water	log Pow: -0.414
Relative vapour density	no data available
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions
no data available

Conditions to avoid
Heat, flames and sparks.

Materials to avoid
Strong oxidizing agents

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx)
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
no data available

Inhalation LC50
no data available

Dermal LD50
no data available

Other information on acute toxicity
no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitization
Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

Germ cell mutagenicity
no data available

Carcinogenicity

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

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

Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Conditions for safe storage
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. Air sensitive.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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

Eye protection
Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

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

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

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	clear, liquid
Colour	light yellow

Safety data

pH	no data available
Melting point/freezing point	no data available
Boiling point	193 °C (379 °F) at 1,013 hPa (760 mmHg)
Flash point	82 °C (180 °F) - closed cup
Ignition temperature	298 °C (568 °F)
Autoignition temperature	no data available
Lower explosion limit	no data available

Product
Contact a licensed professional waste disposal service to dispose of this material. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 2735 Class: 8 Packing group: I
Proper shipping name: Polyamines, liquid, corrosive, n.o.s. (2-Methylpentane-1,5-diamine)
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 2735 Class: 8 Packing group: I EMS-No: F-A, S-B
Proper shipping name: POLYAMINES, LIQUID, CORROSIVE, N.O.S. (2-Methylpentane-1,5-diamine)
Marine pollutant: No

IATA
UN number: 2735 Class: 8 Packing group: I
Proper shipping name: Polyamines, liquid, corrosive, n.o.s. (2-Methylpentane-1,5-diamine)

15. REGULATORY INFORMATION

OSHA Hazards
Combustible Liquid, Harmful by ingestion., Corrosive

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

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

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
2-Methylpentane-1,5-diamine	15520-10-2	

New Jersey Right To Know Components

	CAS-No.	Revision Date
2-Methylpentane-1,5-diamine	15520-10-2	

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

16. OTHER INFORMATION

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

carcinogen or potential carcinogen by ACGIH.

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

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

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
no data available

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Ingestion	May be harmful if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin burns.
Eyes	Causes eye burns.

Signs and Symptoms of Exposure
Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea

Synergistic effects
no data available

Additional Information
RTECS: SA0248500

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

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

NFPA Rating

Health hazard:	3
Fire:	3
Reactivity Hazard:	0

Potential Health Effects

Inhalation	May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Skin	Toxic if absorbed through skin. Causes skin burns.
Eyes	Causes eye burns.
Ingestion	Toxic if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : 3-Methylpyridine

Formula : C_6H_7N

Molecular Weight : 93.13 g/mol

Component		Concentration
3-Methylpyridine		
CAS-No.	108-99-6	-
EC-No.	203-636-9	

4. FIRST AID MEASURES

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

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

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

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

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Suitable extinguishing media
For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx)

Further information
Use water spray to cool unopened containers.

SIGMA-ALDRICH sigma-aldrich.com

Material Safety Data Sheet

Version 4.1
Revision Date 01/19/2012
Print Date 01/13/2013

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	:	3-Picoline
Product Number	:	P42053
Brand	:	Aldrich
Supplier	:	Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	:	+1 800-325-5832
Fax	:	+1 800-325-5052
Emergency Phone # (For both supplier and manufacturer)	:	(314) 776-6555
Preparation Information	:	Sigma-Aldrich Corporation Product Safety - Americas Region 1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Flammable liquid, Target Organ Effect, Toxic by ingestion, Toxic by skin absorption, Corrosive

Target Organs
Liver, Kidney

GHS Classification
Flammable liquids (Category 3)
Acute toxicity, Oral (Category 4)
Acute toxicity, Inhalation (Category 4)
Acute toxicity, Dermal (Category 3)
Skin corrosion (Category 1B)
Serious eye damage (Category 1)

GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H226	Flammable liquid and vapour.
H302 + H332	Harmful if swallowed or if inhaled
H311	Toxic in contact with skin.
H314	Causes severe skin burns and eye damage.

Precautionary statement(s)

P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER or doctor/ physician.

HMIS Classification

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	clear, liquid
Colour	light yellow

Safety data

pH	no data available
Melting point/freezing point	Melting point/range: -19 °C (-2 °F) - lit.
Boiling point	144 °C (291 °F) - lit.
Flash point	37 °C (99 °F) - closed cup
Ignition temperature	538 °C (1,000 °F)
Autoignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	5.9 hPa (4.4 mmHg) at 20 °C (68 °F)
Density	0.957 g/cm3 at 25 °C (77 °F)
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapour density	3.22 - (Air = 1.0)
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions

Vapours may form explosive mixture with air.

Conditions to avoid
hygroscopic
Heat, flames and sparks.

Materials to avoid
acids, Acid chlorides, Oxidizing agents, Chloroformates

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx)
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
LD50 Oral - rat - 400 mg/kg

Inhalation LC50
Dermal LD50

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Conditions for safe storage
Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

hygroscopic

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
3-Methylpyridine	108-99-6	TWA	2 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
Remarks	Skin			
		STEL	5 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
	Skin			

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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

Eye protection
Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin and body protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Hygiene measures
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Toxicity

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - 144 mg/l - 96 h

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 2313 Class: 3 Packing group: III
Proper shipping name: Picolines
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 2313 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: PICOLINES
Marine pollutant: No

IATA
UN number: 2313 Class: 3 Packing group: III
Proper shipping name: Picolines

15. REGULATORY INFORMATION

OSHA Hazards
Flammable liquid, Target Organ Effect, Toxic by ingestion, Toxic by skin absorption, Corrosive

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

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

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

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
3-Methylpyridine	108-99-6	

LD50 Dermal - guinea pig - 1,000 mg/kg

Other information on acute toxicity
no data available

Skin corrosion/irritation
Skin - rabbit - Severe skin irritation - 24 h

Serious eye damage/eye irritation
Eyes - rabbit - Severe eye irritation - 24 h

Respiratory or skin sensitization
no data available

Germ cell mutagenicity
no data available

Carcinogenicity

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

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

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

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

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
no data available

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Ingestion	Toxic if swallowed.
Skin	Toxic if absorbed through skin. Causes skin burns.
Eyes	Causes eye burns.

Signs and Symptoms of Exposure
Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea

Synergistic effects
no data available

Additional Information
RTECS: TJ5000000

12. ECOLOGICAL INFORMATION

New Jersey Right To Know Components

	CAS-No.	Revision Date
3-Methylpyridine	108-99-6	

California Prop. 65 Components

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

16. OTHER INFORMATION

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Physical hazards: 0

NFPA Rating

Health hazard: 2
Fire: 1
Reactivity Hazard: 0

Potential Health Effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.
Ingestion	May be harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : Nicotinic acid amide
Vitamin B3
Pyridine-3-carboxylic acid amide
Vitamin PP
Niacinamide
Nicotinamide

Formula : C6H6N2O
Molecular Weight : 122.12 g/mol

Component		Concentration
Nicotinamide		
CAS-No.	98-92-0	-
EC-No.	202-713-4	

4. FIRST AID MEASURES

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

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

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

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

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

5. FIREFIGHTING MEASURES

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

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx)

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

Environmental precautions
Do not let product enter drains.

Supelco - 47865-U Page 2 of 7

SIGMA-ALDRICH sigma-aldrich.com

Material Safety Data Sheet

Version 4.6
Revision Date 11/13/2012
Print Date 01/13/2013

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Nicotinamide (Niacinamide)

Product Number : 47865-U
Brand : Supelco

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

Telephone : +1 800-325-5832
Fax : +1 800-325-5052
Emergency Phone # (For both supplier and manufacturer) : (314) 776-6555
Preparation Information : Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Target Organ Effect, Irritant

Target Organs

Kidney, Eyes, Liver

GHS Classification
Acute toxicity, Oral (Category 5)
Skin irritation (Category 2)
Eye irritation (Category 2A)
Specific target organ toxicity - single exposure (Category 3)

GHS Label elements, including precautionary statements

Pictogram 

Signal word Warning

Hazard statement(s)

H303	May be harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

Precautionary statement(s)

P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

HMIS Classification

Health hazard: 2
Chronic Health Hazard: *
Flammability: 1

Supelco - 47865-U Page 1 of 7

Safety data

pH	no data available
Melting point/freezing point	Melting point/range: 128 - 131 °C (262 - 268 °F) - lit.
Boiling point	no data available
Flash point	150 °C (302 °F) - closed cup
Ignition temperature	no data available
Autoignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	no data available
Density	no data available
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapour density	no data available
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions
no data available

Conditions to avoid
no data available

Materials to avoid
Strong oxidizing agents

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx)
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
LD50 Oral - rat - 3,500 mg/kg

Inhalation LC50
Dermal LD50
no data available

Other information on acute toxicity
no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation

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

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Conditions for safe storage
Keep container tightly closed in a dry and well-ventilated place.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection
For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator.For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: > 480 min
Material tested:Dermatril® (Aldrich Z677272, Size M)

Splash protection
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: > 30 min
Material tested:Dermatril® (Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an Industrial Hygienist familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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

Skin and body protection
impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

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

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	crystalline
Colour	white

PBT and vPvB assessment
no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

OSHA Hazards
Target Organ Effect, Irritant

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

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

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

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Nicotinamide	98-92-0	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Nicotinamide	98-92-0	

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

16. OTHER INFORMATION

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

no data available

Respiratory or skin sensitization
no data available

Germ cell mutagenicity
no data available

Carcinogenicity

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

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	May be harmful if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.

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

Synergistic effects
no data available

Additional Information
RTECS: QS3675000

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

Health hazard: 0
Fire: 4
Reactivity Hazard: 0

Potential Health Effects

Inhalation	May be harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.
Skin	May be harmful if absorbed through skin. May cause skin irritation.
Eyes	May cause eye irritation.
Ingestion	May be harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : Ethene

Formula : C_2H_4

Molecular Weight : 28.05 g/mol

Component		Concentration
Ethylene		
CAS-No.	74-85-1	-
EC-No.	200-815-3	
Index-No.	601-010-00-3	

4. FIRST AID MEASURES

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

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

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

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

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Conditions of flammability
Flammable in the presence of an oxidizing gas (eg air), a source of ignition, and when the concentration of the gas is between the lower and upper explosive limits. Keep away from heat/sparks/open flame/hot surface/oxidizing gas. No smoking.

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

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

SIGMA-ALDRICH sigma-aldrich.com

Material Safety Data Sheet
Version 3.4
Revision Date 10/29/2012
Print Date 03/19/2013

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	: Ethylene
Product Number	: 03484
Brand	: Fluka
Supplier	: Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	: +1 800-325-5832
Fax	: +1 800-325-5052
Emergency Phone # (For both supplier and manufacturer)	: (314) 776-6555
Preparation Information	: Sigma-Aldrich Corporation Product Safety - Americas Region 1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Flammable gas, Compressed Gas, Target Organ Effect

Target Organs

Central nervous system

GHS Classification
Flammable gases (Category 1)
Gases under pressure (Liquefied gas)
Specific target organ toxicity - single exposure (Category 3)

GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H220	Extremely flammable gas.
H280	Contains gas under pressure; may explode if heated.
H336	May cause drowsiness or dizziness.

Precautionary statement(s)

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P410 + P403	Protect from sunlight. Store in a well-ventilated place.

HMIS Classification
Health hazard: 0
Chronic Health Hazard: *
Flammability: 4
Physical hazards: 3

NFPA Rating

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

Skin and body protection
impervious clothing, Flame retardant antistatic protective clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

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

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	Liquefied gas
Colour	no data available

Safety data

pH	no data available
Melting point/freezing point	Melting point/range: -169 °C (-272 °F) - lit.
Boiling point	-104 °C (-155 °F) - lit.
Flash point	-100 °C (-148 °F) - closed cup
Ignition temperature	450 °C (842 °F)
Autoignition temperature	no data available
Lower explosion limit	2.7 %(V)
Upper explosion limit	36 %(V)
Vapour pressure	35,504.3 hPa (26,630.4 mmHg) at 20 °C (68 °F)
Density	no data available
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapour density	0.97 - (Air = 1.0)
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions
no data available

Conditions to avoid
Heat, flames and sparks. Extremes of temperature and direct sunlight.

Materials to avoid
Strong oxidizing agents, Carbon tetrachloride, Chlorine, Copper, Vinyl compounds

Personal precautions
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up
Clean up promptly by sweeping or vacuum.

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid inhalation of vapour or mist.
Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Conditions for safe storage
Keep container tightly closed in a dry and well-ventilated place.

Contents under pressure.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
Ethylene	74-85-1	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
Remarks	Asphyxia Not classifiable as a human carcinogen			

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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

Immersion protection
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: > 480 min
Material tested:Vitoject® (Aldrich Z677698, Size M)

Splash protection
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: > 30 min
Material tested:Camatril® (Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 873000, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an Industrial Hygienist familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.
Ingestion	May be harmful if swallowed.
Skin	May be harmful if absorbed through skin. May cause skin irritation.
Eyes	May cause eye irritation.

Signs and Symptoms of Exposure
Nausea, Dizziness, Headache, narcosis, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Synergistic effects
no data available

Additional Information
RTECS: KU5340000

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1962 Class: 2.1
Proper shipping name: Ethylene
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 1962 Class: 2.1 EMS-No: F-D, S-U
Proper shipping name: ETHYLENE
Marine pollutant: No

IATA
UN number: 1962 Class: 2.1
Proper shipping name: Ethylene

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
no data available

Inhalation LC50
no data available

Dermal LD50
no data available

Other information on acute toxicity
no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitization
no data available

Germ cell mutagenicity

no data available

Carcinogenicity

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

IARC:	3 - Group 3: Not classifiable as to its carcinogenicity to humans (Ethylene)
NTP:	No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA:	No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

IATA Passenger: Not permitted for transport

15. REGULATORY INFORMATION

OSHA Hazards
Flammable gas, Compressed Gas, Target Organ Effect

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

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Ethylene	74-85-1	2007-07-01

SARA 311/312 Hazards
Fire Hazard, Sudden Release of Pressure Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Ethylene	74-85-1	2007-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Ethylene	74-85-1	2007-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Ethylene	74-85-1	2007-07-01

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

16. OTHER INFORMATION

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Physical hazards: 0

NFPA Rating
Health hazard: 2
Fire: 2
Reactivity Hazard: 0

Potential Health Effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Skin	Harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.
Ingestion	Harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : Nicotinonitrile
Nicotinic acid nitrile
3-Cyanopyridine

Formula : $C_6H_4N_2$
Molecular Weight : 104.11 g/mol

Component		Concentration
Nicotinonitrile		
CAS-No.	100-54-9	-
EC-No.	202-863-0	

4. FIRST AID MEASURES

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

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

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

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

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

5. FIREFIGHTING MEASURES

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

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx), Hydrogen cyanide (hydrocyanic acid)

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

Environmental precautions
Do not let product enter drains.

SIGMA-ALDRICH sigma-aldrich.com

Material Safety Data Sheet

Version 4.1
Revision Date 01/15/2013
Print Date 02/05/2013

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : 3-Pyridinecarbonitrile

Product Number : C94807
Brand : Aldrich

Supplier : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA
Telephone : +1 800-325-5832
Fax : +1 800-325-5052
Emergency Phone # (For both supplier and manufacturer) : (314) 776-6555
Preparation Information : Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Target Organ Effect, Harmful by ingestion., Irritant

Target Organs

Liver, Kidney

GHS Classification
Acute toxicity, Oral (Category 4)
Skin irritation (Category 2)
Eye irritation (Category 2A)
Specific target organ toxicity - single exposure (Category 3)

GHS Label elements, including precautionary statements

Pictogram 

Signal word Warning

Hazard statement(s)

H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

Precautionary statement(s)

P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

HMIS Classification
Health hazard: 2
Chronic Health Hazard: *
Flammability: 0

Safety data

pH	6.5 at 25 °C (77 °F)
Melting point/freezing point	Melting point/range: 48 - 52 °C (118 - 126 °F) - lit.
Boiling point	201 °C (394 °F) - lit.
Flash point	84 °C (183 °F) - closed cup
Ignition temperature	no data available
Auto-ignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	0.395 hPa (0.296 mmHg) at 25 °C (77 °F)
Density	1.159 g/cm3 1.080 g/cm3 at 50 °C (122 °F)
Water solubility	100 g/l at 20 °C (68 °F) - soluble
Partition coefficient: n-octanol/water	log Pow: 0.36
Relative vapor density	no data available
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions
no data available

Conditions to avoid
no data available

Materials to avoid
Strong oxidizing agentsStrong oxidizing agents, Strong acids, Strong bases, Strong reducing agents

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx), Hydrogen cyanide (hydrocyanic acid)
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
LD50 Oral - rat - 1,185 mg/kg
Remarks: Liver:Other changes. Kidney, Ureter, Bladder:Other changes.

Inhalation LC50
no data available

Dermal LD50
no data available

Other information on acute toxicity
no data available

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

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Conditions for safe storage
Keep container tightly closed in a dry and well-ventilated place.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection
For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator.For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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

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

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

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	crystalline
Colour	beige

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects
no data available

13. DISPOSAL CONSIDERATIONS

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

OSHA Hazards
Target Organ Effect, Harmful by ingestion., Irritant

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

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

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

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Nicotinonitrile	100-54-9	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Nicotinonitrile	100-54-9	

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

16. OTHER INFORMATION

Further information

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitization
no data available

Germ cell mutagenicity
no data available

Carcinogenicity

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

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

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

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

Reproductive toxicity

no data available

Teratogenicity
no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	Harmful if swallowed.
Skin	Harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.

Signs and Symptoms of Exposure
Central nervous system depression, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Synergistic effects
no data available

Additional Information
RTECS: QT3030000

12. ECOLOGICAL INFORMATION

Toxicity
no data available

Persistence and degradability
no data available

Fire:	3
Reactivity Hazard:	0

Potential Health Effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.
Ingestion	May be harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : 3-Pipecoline
β-Pipecoline

Formula : $C_6H_{13}N$
Molecular Weight : 99.17 g/mol

Component		Concentration
3-Methylpiperidine		
CAS-No.	626-56-2	-
EC-No.	210-953-6	

4. FIRST AID MEASURES

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

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

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

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

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Suitable extinguishing media
For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx)

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Aldrich - M73001 Page 2 of 6

SIGMA-ALDRICH

sigma-aldrich.com

Material Safety Data Sheet

Version 4.1
Revision Date 11/09/2011
Print Date 01/13/2013

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	:	3-Methylpiperidine
Product Number	:	M73001
Brand	:	Aldrich
Supplier	:	Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	:	+1 800-325-5832
Fax	:	+1 800-325-5052
Emergency Phone # (For both supplier and manufacturer)	:	(314) 776-6555
Preparation Information	:	Sigma-Aldrich Corporation Product Safety - Americas Region 1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Flammable liquid, Irritant

GHS Classification
Flammable liquids (Category 2)
Skin irritation (Category 2)
Eye irritation (Category 2A)
Specific target organ toxicity - single exposure (Category 3)

GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)	
H225	Highly flammable liquid and vapour.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

Precautionary statement(s)	
P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

HMIS Classification

Health hazard:	2
Flammability:	3
Physical hazards:	0

NFPA Rating

Health hazard:	2

Aldrich - M73001 Page 1 of 6

Upper explosion limit	no data available
Vapour pressure	no data available
Density	0.845 g/cm3 at 25 °C (77 °F)
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapour density	no data available
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions

Vapours may form explosive mixture with air.

Conditions to avoid
Heat, flames and sparks. Extremes of temperature and direct sunlight.

Materials to avoid
acids, Acid chlorides, Acid anhydrides, Strong oxidizing agents, Carbon dioxide (CO2)

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx)
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
no data available

Inhalation LC50
Dermal LD50
no data available

Other information on acute toxicity
no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitization
no data available

Germ cell mutagenicity
no data available

Carcinogenicity

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

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

Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Conditions for safe storage
Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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

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

Skin and body protection
impervious clothing, Flame retardant antistatic protective clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

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

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	clear, liquid
Colour	light yellow

Safety data

pH	no data available
Melting point/freezing point	no data available
Boiling point	125 - 126 °C (257 - 259 °F) at 1,017 hPa (763 mmHg) - lit.
Flash point	21 °C (70 °F) - closed cup
Ignition temperature	no data available
Autoignition temperature	no data available
Lower explosion limit	no data available

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1993 Class: 3 Packing group: II
Proper shipping name: Flammable liquids, n.o.s. (3-Methylpiperidine)
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 1993 Class: 3 Packing group: II EMS-No: F-E, S-E
Proper shipping name: FLAMMABLE LIQUID, N.O.S. (3-Methylpiperidine)
Marine pollutant: No

IATA
UN number: 1993 Class: 3 Packing group: II
Proper shipping name: Flammable liquid, n.o.s. (3-Methylpiperidine)

15. REGULATORY INFORMATION

OSHA Hazards
Flammable liquid, Irritant

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

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

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
3-Methylpiperidine	626-56-2	

New Jersey Right To Know Components

	CAS-No.	Revision Date
3-Methylpiperidine	626-56-2	

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

16. OTHER INFORMATION

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Co., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.

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

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	May be harmful if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.

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

Synergistic effects
no data available

Additional Information
RTECS: Not available

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

HMIS Classification

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical hazards:	0

NFPA Rating

Health hazard:	2
Fire:	0
Reactivity Hazard:	0

Potential Health Effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.
Ingestion	May be harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : Diphyl

Component		Classification	Concentration
Diphenyl ether			
CAS-No.	101-84-8	Eye Dam. 1; H318	70 - 90 %
EC-No.	202-981-2		
Biphenyl			
CAS-No.	92-52-4	Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; Aquatic Acute 1; Aquatic Chronic 1; H315, H319, H335, H410	10 - 30 %
EC-No.	202-163-5		
Index-No.	601-042-00-8		

For the full text of the H-Statements and R-Phrases mentioned in this Section, see Section 16

4. FIRST AID MEASURES

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

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

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

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

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

5. FIREFIGHTING MEASURES

Conditions of flammability
Not flammable or combustible.

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

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides

SIGMA-ALDRICH sigma-aldrich.com

Material Safety Data Sheet
Version 4.4
Revision Date 10/10/2012
Print Date 03/19/2013

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	: Dowtherm® A
Product Number	: 44570
Brand	: Aldrich
Supplier	: Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	: +1 800-325-5832
Fax	: +1 800-325-5052
Emergency Phone # (For both supplier and manufacturer)	: (314) 776-6555
Preparation Information	: Sigma-Aldrich Corporation Product Safety - Americas Region 1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Target Organ Effect, Irritant, Mutagen

Target Organs
Liver, Kidney, Spleen., Thyroid, Central nervous system, Peripheral nervous system.

GHS Classification
Acute toxicity, Oral (Category 5)
Skin irritation (Category 2)
Serious eye damage (Category 1)
Specific target organ toxicity - single exposure (Category 3)
Acute aquatic toxicity (Category 1)

GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H303	May be harmful if swallowed.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H335	May cause respiratory irritation.
H400	Very toxic to aquatic life.

Precautionary statement(s)

P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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

Eye protection
Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

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

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

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	clear, liquid
Colour	light yellow

Safety data

pH	no data available
Melting point/freezing point	Melting point/range: 12 - 14 °C (54 - 57 °F)
Boiling point	no data available
Flash point	no data available
Ignition temperature	no data available
Autoignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	no data available
Density	1.063 g/cm3 at 20 °C (68 °F)
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapour density	no data available
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

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

Methods and materials for containment and cleaning up
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Conditions for safe storage
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
Diphenyl ether	101-84-8	TWA	1 ppm	USA. ACGIH Threshold Limit Values (TLV)
Remarks	Eye & Upper Respiratory Tract irritation Nausea			
		STEL	2 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Eye & Upper Respiratory Tract irritation Nausea			
		TWA	1 ppm 7 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
	The value in mg/m3 is approximate.			
		TWA	1 ppm 7 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	1 ppm 7 mg/m3	USA. NIOSH Recommended Exposure Limits
Biphenyl	92-52-4	TWA	0.2 ppm	USA. ACGIH Threshold Limit Values (TLV)
Remarks	Pulmonary function			
		TWA	0.2 ppm 1 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	0.2 ppm 1 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
	The value in mg/m3 is approximate.			
		TWA	0.2 ppm 1 mg/m3	USA. NIOSH Recommended Exposure Limits

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	May be harmful if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.

Signs and Symptoms of Exposure
prolonged or repeated exposure can cause:, Gastrointestinal disturbance, Dermatitis, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Synergistic effects
no data available

Additional Information
RTECS: Not available

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
UN number: 3082 Class: 9 Packing group: III EMS-No: F-A, S-F
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Diphenyl ether)
Marine pollutant: Marine pollutant

IATA
UN number: 3082 Class: 9 Packing group: III
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (Diphenyl ether)

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions
no data available

Conditions to avoid
no data available

Materials to avoid
Strong oxidizing agents

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
no data available

Inhalation LC50
no data available

Dermal LD50
no data available

Other information on acute toxicity
no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
Eyes: no data available

Respiratory or skin sensitization
no data available

Germ cell mutagenicity
no data available

Carcinogenicity

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

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
no data available

Further information
EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

15. REGULATORY INFORMATION

OSHA Hazards
Target Organ Effect, Irritant, Mutagen

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

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Biphenyl	92-52-4	2007-07-01

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

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Diphenyl ether	101-84-8	2007-03-01
Biphenyl	92-52-4	2007-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Diphenyl ether	101-84-8	2007-03-01
Biphenyl	92-52-4	2007-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Diphenyl ether	101-84-8	2007-03-01
Biphenyl	92-52-4	2007-07-01

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

16. OTHER INFORMATION

Text of H-code(s) and R-phrase(s) mentioned in Section 3

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Eye Dam.	Serious eye damage
Eye Irrit.	Eye irritation
H315	Causes skin irritation.
H318	Causes serious eye damage.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H410	Very toxic to aquatic life with long lasting effects.
Skin Irrit.	Skin irritation
STOT SE	Specific target organ toxicity - single exposure

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

DOWTHERM A
Synthetic Organic Heat Transfer Fluid

Saturated Vapor Properties of DOWTHERM A Fluid (SI Units)

Temp. °C	Vapor Pressure bar	Liquid Enthalpy kJ/kg	Latent Heat kJ/kg	Vapor Enthalpy kJ/kg	Vapor Density kg/m³	Vapor Viscosity mPa·s	Vapor Thermal Cond. W/mK	Z_{vapor}	Specific Heat (c_p) kJ/kg K	Ratio of Specific Heats c_p/c_v
15	0.00	4.9	407.2	412.1		0.0054	0.0075	1.000	1.044	1.050
65	0.00	88.1	380.9	469.1	0.0040	0.0063	0.0104	1.000	1.227	1.043
105	0.01	158.1	362.7	520.9	0.0341	0.0071	0.0129	0.999	1.366	1.038
155	0.06	251.2	341.5	592.7	0.2583	0.0080	0.0163	0.995	1.528	1.035
205	0.28	351.2	320.2	671.5	1.179	0.0090	0.0200	0.982	1.681	1.034
255	0.97	458.2	297.4	755.6	3.831	0.0100	0.0238	0.954	1.829	1.036
305	2.60	572.2	271.5	843.6	9.896	0.0110	0.0279	0.908	1.976	1.042
355	5.80	693.1	240.6	933.8	22.03	0.0122	0.0322	0.838	2.133	1.057
405	11.32	822.0	201.7	1023.7	45.17	0.0138	0.0368	0.740	2.333	1.094

Saturated Vapor Properties of DOWTHERM A Fluid (English Units)

Temp. °F	Vapor Pressure psia	Liquid Enthalpy Btu/lb	Latent Heat Btu/lb	Vapor Enthalpy Btu/lb	Vapor Density lb/ft³	Vapor Viscosity cP	Vapor Thermal Cond. Btu/hr ft²(°F/ft)	Z_{vapor}	Specific Heat (c_p) Btu/lb °F	Ratio of Specific Heats c_p/c_v
60	0.000	2.5	175.1	177.6		0.0054	0.0044	1.000	0.250	1.050
120	0.003	26.2	167.3	193.5		0.0060	0.0055	1.000	0.279	1.045
300	0.64	103.0	148.0	251.1	0.0130	0.0079	0.0092	0.996	0.361	1.035
360	2.03	131.1	142.0	273.1	0.0388	0.0086	0.0106	0.989	0.385	1.034
420	5.38	160.6	135.8	296.3	0.0967	0.0092	0.0120	0.977	0.409	1.034
480	12.25	191.4	129.2	320.5	0.2100	0.0098	0.0135	0.959	0.433	1.035
540	24.72	223.5	122.1	345.5	0.4102	0.0105	0.0150	0.932	0.456	1.039
600	45.31	256.9	114.2	371.1	0.7389	0.0113	0.0166	0.895	0.480	1.045
660	76.89	291.7	105.3	397.0	1.254	0.0121	0.0183	0.848	0.505	1.055
720	122.7	327.9	95.0	422.9	2.045	0.0130	0.0200	0.789	0.534	1.073
780	186.4	365.9	82.5	448.4	3.270	0.0142	0.0219	0.714	0.571	1.108

For further information, call...

In the United States and Canada: 1-800-447-4369 • FAX: 1-989-832-1465

In Europe: +32 3 450 2240 • FAX: +32 3 450 2815

In the Pacific: +886 22 547 8731 • FAX: +886 22 713 0092

In other Global Areas: 1-989-832-1560 • FAX: 1-989-832-1465

www.dowtherm.com

Published November 2001

Printed in U.S.A.

NA/LA/Pacific: Form No. 176-01463-1101 AMS
Europe: CH-153-307-E-1101

Product Information

DOWTHERM A

Synthetic Organic Heat Transfer Fluid — Liquid and Vapor Phase Data

DOWTHERM* A heat transfer fluid is a eutectic mixture of two very stable compounds, biphenyl ($C_{12}H_{10}$) and diphenyl oxide ($C_{12}H_{10}O$). These compounds have practically the same vapor pressures, so the mixture can be handled as if it were a single compound. DOWTHERM A fluid may be used in systems employing either liquid phase or vapor phase heating.

Recommended use temperature range:
Liquid phase: 15°C (60°F) to 400°C (750°F)
Vapor phase: 257°C (495°F) to 400°C (750°F)

Suitable applications: Indirect heat transfer

For health and safety information for this product, contact your Dow sales representative or call the number for your area on the second page of this sheet for a Material Safety Data Sheet (MSDS).

Typical Properties of DOWTHERM A Fluid†

Composition: Diphenyl Oxide/Biphenyl Blend

Color: Clear to Light Yellow

Property	SI Units	English Units
Freeze Point	12.0°C	53.6°F
Atmospheric Boiling Point	257.1°C	494.8°F
Flash Point[1]	113°C	236°F
Fire Point[2]	118°C	245°F
Autoignition Temperature[3]	599°C	1110°F
Density @ 25°C (75°F)	1056 kg/m³	66.0 lb/ft³
Surface Tension in Air @		
20°C (68°F)	40.1 Dynes/cm	40.1 Dynes/cm
40°C (104°F)	37.6 Dynes/cm	37.6 Dynes/cm
60°C (140°F)	35.7 Dynes/cm	35.7 Dynes/cm
Estimated Critical Temperature	497°C	927°F
Estimated Critical Pressure	31.34 bar	30.93 atm
Estimated Critical Volume	3.17 l/kg	0.0508 ft³/lb
Average Molecular Weight		166.0
Heat of Combustion	36,053 kJ/kg	15,500 Btu/lb

† Not to be construed as specifications
[1] SETA
[2] C.O.C.
[3] ASTM E659-78

Saturated Liquid Properties of DOWTHERM A Fluid (SI units)

Temp. °C	Vapor Pressure bar	Viscosity mPa sec	Specific Heat kJ/kg K	Thermal Cond. W/mK	Density kg/m³
15	0.00	5.00	1.558	0.1395	1063.5
65	0.00	1.58	1.701	0.1315	1023.7
105	0.01	0.91	1.814	0.1251	990.7
155	0.06	0.56	1.954	0.1171	947.8
205	0.28	0.38	2.093	0.1091	902.5
255	0.97	0.27	2.231	0.1011	854.0
305	2.60	0.20	2.373	0.0931	801.3
355	5.80	0.16	2.527	0.0851	742.3
405	11.32	0.12	2.725	0.0771	672.5

Saturated Liquid Properties of DOWTHERM A Fluid (English units)

Temp. °F	Vapor Pressure psia	Viscosity cP	Specific Heat Btu/lb °F	Thermal Cond. Btu/hr ft²(°F/ft)	Density lb/ft³
60	0.000	4.91	0.373	0.0805	66.37
120	0.003	2.12	0.396	0.0775	64.72
180	0.028	1.22	0.418	0.0744	63.03
240	0.16	0.81	0.441	0.0713	61.30
300	0.64	0.59	0.463	0.0682	59.51
360	2.03	0.45	0.485	0.0651	57.65
420	5.38	0.35	0.507	0.0620	55.72
480	12.25	0.28	0.529	0.0590	53.70
540	24.72	0.23	0.552	0.0559	51.57
600	45.31	0.19	0.575	0.0528	49.29
660	76.89	0.16	0.599	0.0497	46.82
720	122.7	0.14	0.627	0.0466	44.08
780	186.4	0.12	0.665	0.0436	40.93

*Trademark of The Dow Chemical Company

	present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER or doctor/ physician.
P410 + P403	Protect from sunlight. Store in a well-ventilated place.

HMIS Classification

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

NFPA Rating

Health hazard:	3
Fire:	0
Reactivity Hazard:	0

Potential Health Effects

Inhalation	May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Skin	May be harmful if absorbed through skin. Causes skin burns.
Eyes	Causes eye burns.
Ingestion	May be harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Formula : H_3N

Molecular Weight : 17.03 g/mol

Component		Concentration
Ammonia, anhydrous		
CAS-No.	7664-41-7	-
EC-No.	231-635-3	
Index-No.	007-001-00-5	

4. FIRST AID MEASURES

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

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

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

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

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Conditions of flammability
Not flammable or combustible.

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

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

SIGMA-ALDRICH

sigma-aldrich.com

Material Safety Data Sheet

Version 3.4
Revision Date 12/05/2012
Print Date 01/13/2013

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	:	Ammonia
Product Number	:	294993
Brand	:	Aldrich
Supplier	:	Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	:	+1 800-325-5832
Fax	:	+1 800-325-5052
Emergency Phone # (For both supplier and manufacturer)	:	(314) 776-6555
Preparation Information	:	Sigma-Aldrich Corporation Product Safety - Americas Region 1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Compressed Gas, Target Organ Effect, Corrosive

Target Organs

Lungs, Central nervous system, Liver, Kidney

GHS Classification
Flammable gases (Category 2)
Gases under pressure (Compressed gas)
Acute toxicity, Inhalation (Category 3)
Skin corrosion (Category 1B)
Serious eye damage (Category 1)
Acute aquatic toxicity (Category 1)

GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H221	Flammable gas.
H280	Contains gas under pressure; may explode if heated.
H314	Causes severe skin burns and eye damage.
H331	Toxic if inhaled.
H400	Very toxic to aquatic life.

Precautionary statement(s)

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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

Full contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash protection
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an Industrial Hygienist familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Eye protection
Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin and body protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Hygiene measures
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	Compressed gas
Colour	no data available

Safety data

pH	no data available
Melting point/freezing point	Melting point/range: -78 °C (-108 °F) - lit.
Boiling point	-33 °C (-27 °F) - lit.
Flash point	132 °C (270 °F) - closed cup
Ignition temperature	651 °C (1,204 °F)
Auto-ignition temperature	no data available
Lower explosion limit	15 %(V)
Upper explosion limit	25 %(V)

Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - nitrogen oxides (NOx)

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

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

Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Conditions for safe storage
Keep container tightly closed in a dry and well-ventilated place.

Contents under pressure.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
Ammonia, anhydrous	7664-41-7	TWA	25 ppm	USA. ACGIH Threshold Limit Values (TLV)
Remarks	Upper Respiratory Tract irritation Eye damage			
		STEL	35 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Upper Respiratory Tract irritation Eye damage			
		STEL	35 ppm 27 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	50 ppm 35 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
	The value in mg/m3 is approximate.			
		TWA	25 ppm 18 mg/m3	USA. NIOSH Recommended Exposure Limits
	Often used in an aqueous solution.			
		ST	35 ppm 27 mg/m3	USA. NIOSH Recommended Exposure Limits
	Often used in an aqueous solution.			

carcinogen or potential carcinogen by ACGIH.

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

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

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
no data available

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.
Ingestion	May be harmful if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin burns.
Eyes	Causes eye burns.

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

Synergistic effects
no data available

Additional Information
RTECS: BO0875000

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Toxicity to daphnia and other aquatic invertebrates	LC50 - Daphnia magna (Water flea) - 25.4 mg/l - 48 h

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life.

Vapour pressure	6,402 hPa (4,802 mmHg) at 15.50 °C (59.90 °F) 8,866 hPa (6,650 mmHg) at 21 °C (70 °F)
Density	0.590 g/cm3
Water solubility	soluble
Partition coefficient: n-octanol/water	no data available
Relative vapor density	0.59 - (Air = 1.0)
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions
no data available

Conditions to avoid
Heat, flames and sparks. Extremes of temperature and direct sunlight.

Materials to avoid
Oxidizing agents, Iron, Zinc, Copper, Silver/silver oxides, Cadmium/cadmium oxides, Alcohols, acids, Halogens, Aldehydes

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - nitrogen oxides (NOx)
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
no data available

Inhalation LC50
LC50 Inhalation - rat - 4 h - 2000 ppm

Dermal LD50
no data available

Other information on acute toxicity
no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitization
no data available

Germ cell mutagenicity
no data available

Carcinogenicity

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

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

no data available

13. DISPOSAL CONSIDERATIONS

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1005 Class: 2.3 (8)
Proper shipping name: Ammonia, anhydrous
Reportable Quantity (RQ): 100 lbs
Marine Pollutant: No
Poison Inhalation Hazard: Hazard zone D

IMDG
UN number: 1005 Class: 2.3 (8) EMS-No: F-C, S-U
Proper shipping name: AMMONIA, ANHYDROUS
Marine Pollutant: No

IATA
UN number: 1005 Class: 2.3 (8)
Proper shipping name: Ammonia, anhydrous
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport

15. REGULATORY INFORMATION

OSHA Hazards
Compressed Gas, Target Organ Effect, Corrosive

SARA 302 Components
The following components are subject to reporting levels established by SARA Title III, Section 302:

	CAS-No.	Revision Date
Ammonia, anhydrous	7664-41-7	2007-03-01

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Ammonia, anhydrous	7664-41-7	2007-03-01

SARA 311/312 Hazards
Sudden Release of Pressure Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Ammonia, anhydrous	7664-41-7	2007-03-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Ammonia, anhydrous	7664-41-7	2007-03-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Ammonia, anhydrous	7664-41-7	2007-03-01

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

16. OTHER INFORMATION

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.