

Abstract
Process Economics Program Report 240
STRATEGIC BUSINESS UNITS OF NYLON 6 AND NYLON 66
(December 2001)

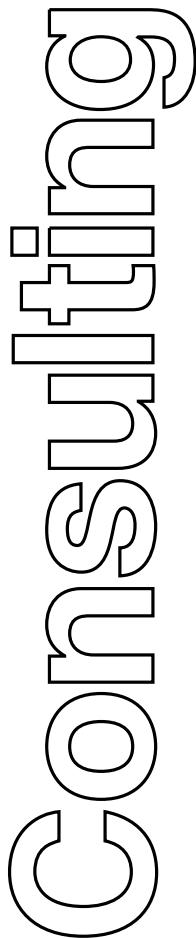
This report presents economics for ten cases of strategic business units (SBUs), five each for the production of nylon 6 and nylon 66 resins. The SBU is an integrated operation, which combines the production of nylon resin with the production of precursor(s). The determination of the configuration of each SBU is based on the information of worldwide production capacities for nylon resins and their precursors. The latter include caprolactam (CAPM) for nylon 6, and adipic acid (ADA) and hexamethylenediamine (HMDA) for nylon 66.

This report presents economics of five processes for the production of CAPM, three processes for the production of ADA and two processes for the production of HMDA along with those of processes producing nylon 6 chips and nylon 66 resins. They are

- Hydroxylamine phosphate (HPO) process, which uses phosphoric acid as hydroxylamine carrier, produces CAPM from phenol.
- Hydroxylamine phosphate (HPO) process, which uses phosphoric acid as hydroxylamine carrier, produces CAPM from cyclohexane.
- Nitric oxide (NO_x) reduction process, which uses hydroxylammonium-ammonium sulfate as hydroxylamine carrier, produces CAPM from cyclohexane.
- CAPM from butadiene via methyl 6-aminocaproate by carboalkoxylation, hydroformylation and reductive ammoniation followed by cyclization with no ammonium sulfate by-product
- CAPM from butadiene via 6-aminocapronitrile by hydrocyanation and partial hydrogenation followed by cyclization; the process produces HMDA as a co-product and no ammonium sulfate by-product.
- ADA from cyclohexane by oxidation process
- ADA from butadiene by carboalkoxylation process
- ADA from benzene by partial hydrogenation process
- HMDA from butadiene by hydrocyanation process
- HMDA from butadiene via 6-aminocapronitrile by hydrocyanation and partial hydrogenation followed by cyclization; the process produces CAPM as co-product and no ammonium sulfate by-product.

This report also presents economics comparison among the SBUs.

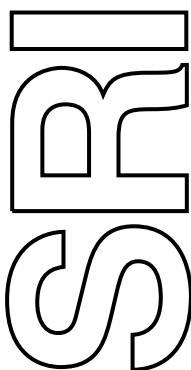
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STRATEGIC BUSINESS UNITS OF NYLON 6 AND NYLON 66

by YU-REN CHIN



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1 INTRODUCTION

This report, PEP Report 240, reviews the technology for producing nylon 6 and nylon 66 resins as well as their precursors. In this report, we present economics of five processes for the production of caprolactam (CAPM), three processes for the production of adipic acid (ADA) and two processes for the production of hexamethylenediamine (HMDA) along with those of processes producing nylon 6 chips and nylon 66 resins. The processes for those precursors are summarized below:

- Hydroxylamine phosphate (HPO) process, which uses phosphoric acid as hydroxylamine carrier, produces CAPM from phenol.
- Hydroxylamine phosphate (HPO) process, which uses phosphoric acid as hydroxylamine carrier, produces CAPM from cyclohexane.
- Nitric oxide reduction process, which uses hydroxylammonium-ammonium sulfate as hydroxylamine carrier, produces CAPM from cyclohexane.
- CAPM from butadiene via methyl 6-aminocaproate by carboalkoxylation, hydroformylation and reductive ammoniation followed by cyclization with no ammonium sulfate by-product
- CAPM from butadiene via 6-aminocapronitrile by hydrocyanation and partial hydrogenation followed by cyclization; the process produces HMDA as co-product and no ammonium sulfate by-product.
- ADA from cyclohexane by the oxidation process
- ADA from butadiene by the carboalkoxylation process
- ADA from benzene by the partial hydrogenation process
- HMDA from butadiene by hydrocyanation process
- HMDA from butadiene via 6-aminocapronitrile by hydrocyanation and partial hydrogenation followed by cyclization; the process produces CAPM as co-product and no ammonium sulfate by-product.

Also presented in this report are ten cases of strategic business units (SBUs), five each for the production of nylon 6 and nylon 66 resins. They are listed below:

- N6-SBU1—Integration of cyclohexane-based NO_x process with continuous process for nylon 6 chips
- N6-SBU2—Integration of cyclohexane-based HPO process with continuous process for nylon 6 chips
- N6-SBU3—Integration of phenol-based HPO process with continuous process for nylon 6 chips
- N6-SBU4—Integration of butadiene-based CAPM process via amino-caproate with continuous process for nylon 6 chips

- N6-SBU5—Integration of butadiene-based CAPM/HMDA process via adiponitrile with continuous process for nylon 6 chips
- N66-SBU1—Integration of cyclohexane-based ADA oxidation process and butadiene-based HMDA hydrocyanation process with continuous process for nylon 66 resins
- N66-SBU2—Integration of Butadiene-based ADA carbalkylation process and butadiene-based HMDA hydrocyanation process with continuous process for nylon 66 resins
- N66-SBU3—Integration of benzene-based ADA process and butadiene-based HMDA hydrocyanation process with continuous process for nylon 66 resins
- N66-SBU4—Integration of cyclohexane-based ADA oxidation process and adiponitrile-based HMDA process with continuous process for nylon 66 resins
- N66-SBU5—Integration of butadiene-based CAPM/HMDA process via adiponitrile with continuous process for nylon 66 resins

Each SBU integrates the production of nylon resin with those of precursor(s). Based on the information of production capacities presented in Section 3 of this report, we determine the configurations of these units, and estimate as well as compare their economics.

2 SUMMARY

World consumption of nylon 6 and nylon 66 in 2000 in the forms of resins and fibers is estimated to be about 6.2 million tons (13.7 billion pounds), of which approximately 60% is accounted for by nylon 66, and up to 40% by nylon 6. The total year-2000 demand for nylon resins in the world major consuming regions, i.e. North America (the United States and Canada), Western Europe, portions of East Asia, was reported at 1.54 million metric tons. With present global economic slowdown, we estimated the total demand for nylon resins in these regions in 2005 at about 1.7 million tons, representing an average annual growth rate of 2%. The total demand for nylon fibers in the above major regions was estimated at about 3.56 million metric tons in 2000. The total demand in 2005 is estimated at 3.9 million metric tons. The major markets for nylon fibers are apparel, home furnishings, and industrial and consumer products. Nylon resins are fabricated into various product forms: blow molding, injection molding, film and sheet, pipe and conduit, wire and cable, fibers, and others.

TECHNICAL ASPECTS

Nylon 6 and Its Precursor

Nylon 6 is commercially produced from CAPM mostly by hydrolytic polymerization process, and, to a less extent, by anionic polymerization process. At present, most of the CAPM is commercially prepared via cyclohexanone, which is derived from cyclohexane by oxidation or from phenol by hydrogenation. The cyclohexanone is then converted to cyclohexanone oxime by one of the following two approaches:

- The hydroxylamine phosphate (HPO) process, which uses phosphoric acid as hydroxylamine carrier, produces CAPM from phenol or cyclohexane as feedstock and less amount of ammonium sulfate than the traditional Raschig process.
- The nitric oxide (NO_x) reduction process, which uses hydroxylammonium-ammonium sulfate as hydroxylamine carrier, produces CAPM from cyclohexane and also less amount of ammonium sulfate.

Recently, two butadiene-based CAPM processes have been developed; one jointly developed by DSM and DuPont, and the other by BASF and DuPont. They are respectively

- CAPM from butadiene via methyl 6-aminocaproate by carboalkoxylation, hydroformylation and reductive ammoniation followed by cyclization
- CAPM from butadiene via 6-aminocapronitrile by hydrocyanation and partial hydrogenation followed by cyclization; the process co-producing HMDA

World total production capacity for CAPM is estimated at about 4.15 million ton/yr of which 31% is accounted for by the producers in Asia Pacific, 26% by the producers in Western Europe, 23% by the producers in North America, and the remainder by the producers in Eastern Europe. Except a few producers with their feedstocks either unknown at the present time or using feedstocks, such as benzene, cyclohexanone and waste carpets, all other CAPM producers have

their feedstocks based on phenol or cyclohexane. About 20% of the total world CAPM production capacity is based on phenol and 56% based on cyclohexane.

Nylon 66 and Its Precursors

Nylon 66 is prepared from ADA and HMDA via nylon salt, which is further polycondensated to nylon resins. Nylon 66 fibers can be made directly from the polycondensated polymer by melt spinning or nylon 66 chips. ADA is produced by oxidation of KA oil (a mixture of cyclohexanone and cyclohexanol), which is prepared either from cyclohexane by oxidation or from phenol by hydrogenation. At present, the majority of ADA production is based on the cyclohexane route. Recently, cyclohexanol is produced from benzene via cyclohexene by partial hydrogenation. The latter is subjected to hydration to produce cyclohexanol, which is then oxidized to ADA similarly as the conventional process. There have been many activities in research development on various processes producing ADA from butadiene. SRI has reviewed these activities in both PEP Report 3B and the present report. Among those processes, we believe that a process, which produces ADA from butadiene by carboalkoxylation, is more commercially viable. In this report we present the following three processes for the production of ADA.

- Adipic acid from cyclohexane by the oxidation process
- Adipic acid from butadiene by the carboalkoxylation process
- Adipic acid from benzene by the partial hydrogenation process

The total production capacity for ADA is estimated at about 5.93 billion lb/yr (2.69 million ton/yr). The production capacity in North America accounts for 44% of the total, which is followed by 35% by the producers in Western Europe, 16% by the producers in Asia Pacific, and the remainder by the producers in Eastern Europe and South America.

Commercially, HMDA is produced by hydrogenation of adiponitrile (ADN), which is mostly prepared from butadiene by hydrocyanation process and is also produced, to a less extent, by electrohydrodimerization process. For many years, HMDA was also produced from adipic acid by reacting with ammonia over a dehydration catalyst. This process is no longer used in the major producing regions in the world. As mentioned earlier, a new technology developed jointly by BASF and DuPont to co-produce HMDA and CAPM by partial hydrogenation of ADN. This process has not been commercially installed. The total production capacity for HMDA is estimated at 3.42 billion lb/yr (1.55 million ton/yr), of which about 57% is located in North America and 33% in Western Europe. Feedstocks for HMDA production include butadiene at 46%, adiponitrile at 33%, and the remainder is acrylonitrile. In this report, we present the economics for the production of HMDA by integrating the process for hydrocyanation of butadiene to the process for hydrogenation of ADN. Also presented are economics for the coproduction of HMDA and CAPM by integrating the process for hydrocyanation of butadiene to the process for partial hydrogenation of ADN.

Strategic Business Units for Nylon Resins

Ten cases of strategic business units (SBUs), five each for the production of nylon 6 and nylon 66 resins are present in this report. The SBU is an integrated operation, which combines the production of nylon resin with the production of precursor(s). The determination of the configuration of each SBU is based on the information of worldwide production capacities for nylon resins and their precursors. They are summarized below:

- N6-SBU1—Integration of cyclohexane-based NOx process with continuous process for nylon 6 chips
- N6-SBU2—Integration of cyclohexane-based HPO process with continuous process for nylon 6 chips
- N6-SBU3—Integration of phenol-based HPO process with continuous process for nylon 6 chips
- N6-SBU4—Integration of butadiene-based CAPM process via amino-caproate with continuous process for nylon 6 chips
- N6-SBU5—Integration of butadiene-based CAPM/HMDA process via adiponitrile with continuous process for nylon 6 chips
- N66-SBU1—Integration of cyclohexane-based ADA oxidation process and butadiene-based HMDA hydrocyanation process with continuous process for nylon 66 resins
- N66-SBU2—Integration of Butadiene-based ADA carbalkylation process and butadiene-based HMDA hydrocyanation process with continuous process for nylon 66 resins
- N66-SBU3—Integration of benzene-based ADA process and butadiene-based HMDA hydrocyanation process with continuous process for nylon 66 resins
- N66-SBU4—Integration of cyclohexane-based ADA oxidation process and adiponitrile-based HMDA process with continuous process for nylon 66 resins
- N66-SBU5—Integration of butadiene-based CAPM/HMDA process via adiponitrile with continuous process for nylon 66 resins

In each of SBU1 through SBU4, the economics of a stand-alone nylon resin plant is also considered. In such a case, the unit prices for the precursors used in the production are derived from precursor plants with greater capacities considered in the configuration. Two alternative cases are considered in each of N6-SBU5 and N66-SBU5. They are:

- Case A – The nylon resin production is combined with its precursor production by integrating half of the capital investment, and raw material and utilities consumption from the CAPM-HMDA plant to those of the nylon resin plant. In such a case, the co-product either HMDA or CAPM is not credited.
- Case B – The nylon resin production is combined with its precursor production by integrating total of the capital investment, and raw material and utilities consumption from the CAPM-HMDA plant to those of the resin plant. In such a case, the co-product either HMDA or CAPM is credited.

COMPARISON OF ECONOMICS

Economics for CAPM Production

Table 2.1 summarizes the capital investment and production costs for the three commercial processes, which produce CAPM via cyclohexanone. The total fixed capital (TFC) for the phenol-based HPO process and the cyclohexane-based NOx process appears very competitive, within a ±10% range. The cyclohexane-based HPO process has the highest total fixed capital among the three processes. In the production costs, the cyclohexane-based NOx process provides lowest production costs among the three processes, mainly due to the low raw material

costs. Although the cyclohexane-based HPO process has the raw material costs 30 % lower than the phenol-based HPO process does, the difference is offset by the high fixed costs due to its high TFC.

Table 2.2 gives the economics for the two butadiene-based CAPM processes, which are commercially viable but have not been commercially installed at this moment. These two processes require high capital investment as compared with the commercial CAPM processes shown in Table 2.1. However, the cheap butadiene cost provides advantage in the production costs, resulting in less than 1 \$/lb for the product value.

Economics for ADA Production

Table 2.3 summarizes the economics for the three ADA processes. The capital investment for the butadiene-based ADA process requires about \$32 million higher than the cyclohexane-based ADA process and about \$6 million higher than the benzene-based ADA process in TFC. In production costs, it has about 6-7 ¢/lb advantage over the other two processes in variable costs. This advantage is reduced to 2-6 ¢/lb due to its high fixed costs.

The variable costs between the cyclohexane-based ADA process and the benzene-based ADA process are competitive, but the latter's relatively high capital investment entails some disadvantage to its fixed costs, resulting in a nearly 4 ¢/lb higher in product value.

Economics for HMDA Production

The economics for the two HMDA processes are given in Table 2.4. No direct economic comparison is possible in this case as two processes have different sizes of production capacity. However, these processes have competitive product values. The credit for CAPM in the HMDA-CAPM co-production process, nevertheless, entails an influential factor on the product value of HMDA. In this case, CAPM is credited at 84 ¢/lb, and a higher credit value for CAPM could proportionally reduce the product value of HMDA.

Economics for Nylon Resin Production

The economics for the production of nylon 6 and nylon 66 resins are listed in Table 2.5. At production capacity of 135 million lb/yr, both capital investment and production costs for nylon 66 resins are slightly lower than those for nylon 6 resins.

Table 2.1
ECONOMICS FOR CAPM PROCESSES VIA CYCLOHEXANE OXIME

ECONOMIC COMPARISON

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

PEP COST INDEX: 624

	CAPM from Phenol by HPO Process	CAPM from Cyclohexane by NOx Process	CAPM from Cyclohexane by HPO Process
PRODUCTION CAPACITY, MILLION LB/YR (THOUSAND METRIC TON/YR)	309 (140)	309 (140)	309 (140)
INVESTMENT (\$ MILLIONS)			
BATTERY LIMITS (BLI)	207.4	205.2	266.3
OFFSITES	<u>142.8</u>	<u>176.1</u>	<u>200.5</u>
TOTAL FIXED CAPITAL (TFC)	350.2	381.3	466.8
PRODUCTION COSTS (¢/LB)			
RAW MATERIALS	48.53	31.05	33.22
BY-PRODUCTS	-3.47	-3.65	-3.60
UTILITIES	<u>8.42</u>	<u>11.91</u>	<u>15.37</u>
VARIABLE COSTS	53.48	39.31	44.99
WORKERS/SHIFT	15	12	15
OPERATING LABOR, @\$33.58/HR	1.43	1.14	1.43
MAINTENANCE LABOR, 3%/YR OF BLI	2.02	1.99	2.59
CONTROL LAB LABOR, 20% OF OPERATING LABOR	<u>0.29</u>	<u>0.23</u>	<u>0.29</u>
LABOR COSTS	3.74	3.36	4.31
MAINTENANCE MATERIALS, 3%/YR OF BLI	2.02	1.99	2.59
OPERATING SUPPLIES, 10%/YR OF OPERATING LABOR	<u>0.14</u>	<u>0.11</u>	<u>0.14</u>
TOTAL DIRECT COSTS	59.38	44.77	52.03
PLANT OVERHEAD, 80% OF LABOR COSTS	2.99	2.69	3.45
TAXES AND INSURANCE, 2%/YR OF TFC	<u>2.27</u>	<u>2.47</u>	<u>3.03</u>
PLANT CASH COSTS	64.64	50.35	58.51
DEPRECIATION, 10%/YR OF TFC	<u>11.35</u>	<u>12.35</u>	<u>15.13</u>
PLANT GATE COSTS	75.99	62.28	73.64
G&A, SALES, RESEARCH	<u>9.00</u>	<u>9.00</u>	<u>9.00</u>
NET PRODUCTION COST	84.99	71.28	82.64
ROI BEFORE TAXES, 25%/YR OF TFC	<u>28.37</u>	<u>30.88</u>	<u>37.82</u>
PRODUCT VALUE	113.36	102.16	120.46

Table 2.2
ECONOMICS FOR BUTADIENE-BASED CAPM PROCESSES

ECONOMIC COMPARISON

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

PEP COST INDEX: 624

	CAPM from Butadiene via 6-Aminocaproate	CAPM & HMDA from Butadiene via Aminocapronitrile
PRODUCTION CAPACITY, MILLION LB/YR (THOUSAND METRIC TON/YR)	300 (136)	330 (150)
INVESTMENT (\$ MILLIONS)		
BATTERY LIMITS (BLI)	232.1	195.7
OFFSITES	<u>162.6</u>	<u>280.9</u>
TOTAL FIXED CAPITAL (TFC)	394.7	476.6
PRODUCTION COSTS (\$/LB)		
RAW MATERIALS	14.71	86.55
BY-PRODUCTS	—	-93.29
UTILITIES	<u>14.61</u>	<u>20.94</u>
VARIABLE COSTS	29.32	14.20
WORKERS/SHIFT	12	12
OPERATING LABOR, @\$33.58/HR	1.18	1.07
MAINTENANCE LABOR, 1.6%/YR OF BLI	2.32	1.78
CONTROL LAB LABOR, 20% OF OPERATING LABOR	<u>0.24</u>	<u>0.21</u>
LABOR COSTS	3.74	3.06
MAINTENANCE MATERIALS, 2.4%/YR OF BLI	2.32	1.78
OPERATING SUPPLIES, 10%/YR OF OPERATING LABOR	<u>0.12</u>	<u>0.11</u>
TOTAL DIRECT COSTS	35.50	19.15
PLANT OVERHEAD, 80% OF LABOR COSTS	2.99	2.45
TAXES AND INSURANCE, 2%/YR OF TFC	<u>2.63</u>	<u>2.89</u>
PLANT CASH COSTS	41.12	24.49
DEPRECIATION, 10%/YR OF TFC	<u>13.16</u>	<u>14.44</u>
PLANT GATE COSTS	54.28	38.93
G&A, SALES, RESEARCH	<u>9.00</u>	<u>9.00</u>
NET PRODUCTION COST	63.28	47.93
ROI BEFORE TAXES, 25%/YR OF TFC	<u>32.89</u>	<u>36.10</u>
PRODUCT VALUE	96.17	84.03

Table 2.3
ADIPIC ACID BY OXIDATION PROCESSES

ECONOMIC COMPARISON

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

PEP COST INDEX: 624

	ADA from Cyclohexane by Oxidation Process	ADA from Butadiene by Carboalkoxylati on Process	ADA from Benzene by Partial Hydrogenation Process
PRODUCTION CAPACITY, MILLION LB/YR (THOUSAND METRIC TON/YR)	300 (136)	300 (136)	300 (136)
INVESTMENT (\$ MILLIONS)			
BATTERY LIMITS (BLI)	158.2	179.8	166.4
OFFSITES	<u>93.7</u>	<u>103.4</u>	<u>110.5</u>
TOTAL FIXED CAPITAL (TFC)	251.9	283.2	276.9
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	23.23	21.90	22.93
BY-PRODUCTS	-3.78	-7.27	-3.35
UTILITIES	<u>6.33</u>	<u>5.03</u>	<u>8.21</u>
VARIABLE COSTS	25.88	19.66	26.79
WORKERS/SHIFT	12	10	10
OPERATING LABOR, @\$33.58/HOUR	1.18	0.98	0.98
MAINTENANCE LABOR, 3%/YR OF BLI	1.58	1.80	1.66
CONTROL LAB LABOR, 20% OF OPERATING LABOR	<u>0.24</u>	<u>0.20</u>	<u>0.20</u>
LABOR COSTS	3.00	2.98	2.84
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.58	1.80	1.66
OPERATING SUPPLIES, 10%/YR OF OPERATING LABOR	<u>0.12</u>	<u>0.10</u>	<u>0.10</u>
TOTAL DIRECT COSTS	30.58	24.54	31.39
PLANT OVERHEAD, 80% OF LABOR COSTS	2.40	2.38	2.27
TAXES AND INSURANCE, 2%/YR OF TFC	<u>1.68</u>	<u>1.89</u>	<u>1.85</u>
PLANT CASH COSTS	34.66	28.81	35.51
DEPRECIATION, 10%/YR OF TFC	<u>8.40</u>	<u>9.44</u>	<u>9.23</u>
PLANT GATE COSTS	43.06	38.25	44.74
G&A, SALES, RESEARCH	<u>7.00</u>	<u>7.00</u>	<u>7.00</u>
NET PRODUCTION COST	50.06	45.25	51.74
ROI BEFORE TAXES, 25%/YR OF TFC	<u>20.99</u>	<u>23.60</u>	<u>23.08</u>
PRODUCT VALUE	71.05	68.85	74.82

Table 2.4
PROCESSES FOR HEXAMETHYLENEDIAMIN FROM BUTADIENE

ECONOMIC COMPARISON		
CAPACITY: 300 MILLION LB/YR (136,000 T/YR)		
PEP COST INDEX: 624		
	HMDA from Butadiene by Hydrocyanation	CAPM & HMDA from Butadiene via Adiponitrile
PRODUCTION CAPACITY, MILLION LB/YR (THOUSAND METRIC TON/YR)	200 (90.7)	330 (150)
INVESTMENT (\$ MILLIONS)		
BATTERY LIMITS (BLI)	95.0	195.7
OFFSITES	<u>62.1</u>	<u>280.9</u>
TOTAL FIXED CAPITAL (TFC)	156.3	476.6
PRODUCTION COSTS (¢/LB)		
RAW MATERIALS	43.27	86.55
BY-PRODUCTS	-1.34	-84.32
UTILITIES	<u>5.69</u>	<u>20.94</u>
VARIABLE COSTS	47.62	23.17
OPERATING LABOR, 12 WORKERS/SHIFT @\$33.58/HR	1.76	1.07
MAINTENANCE LABOR, 1.6%/YR OF BLI	1.43	1.78
CONTROL LAB LABOR, 20% OF OPERATING LABOR	<u>0.35</u>	<u>0.21</u>
LABOR COSTS	3.54	3.06
MAINTENANCE MATERIALS, 2.4%/YR OF BLI	1.43	1.78
OPERATING SUPPLIES, 10%/YR OF OPERATING LABOR	<u>0.18</u>	<u>0.11</u>
TOTAL DIRECT COSTS	52.77	28.12
PLANT OVERHEAD, 80% OF LABOR COSTS	2.83	2.45
TAXES AND INSURANCE, 2%/YR OF TFC	<u>1.56</u>	<u>2.89</u>
PLANT CASH COSTS	57.16	33.46
DEPRECIATION, 10%/YR OF TFC	<u>7.81</u>	<u>14.44</u>
PLANT GATE COSTS	64.97	47.90
G&A, SALES, RESEARCH	<u>9.00</u>	<u>9.00</u>
NET PRODUCTION COST	73.97	56.90
ROI BEFORE TAXES, 25%/YR OF TFC	<u>19.53</u>	<u>36.10</u>
PRODUCT VALUE	93.50	93.00

Table 2.5
PROCESSES FOR NYLON 6 AND NYLON 66

ECONOMIC COMPARISON

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

PEP COST INDEX: 624

	Process 1: Nylon 6 Chips from CAPM by Continuous Process	Process 2: Nylon 66 resin via nylon salt by Continuous Process
PRODUCTION CAPACITY, MILLION LB/YR (THOUSAND METRIC TON/YR)	135 (61.2)	135 (61.2)
INVESTMENT (\$ MILLIONS)		
BATTERY LIMITS (BLI)	52.3	48.2
OFFSITES	<u>38.3</u>	<u>24.5</u>
TOTAL FIXED CAPITAL (TFC)	90.6	72.7
PRODUCTION COSTS (¢/LB)		
RAW MATERIALS	89.75	86.99
BY-PRODUCTS	—	—
UTILITIES	<u>4.39</u>	<u>1.88</u>
VARIABLE COSTS	94.14	88.87
WORKERS/SHIFT	4	5
OPERATING LABOR, @\$33.58/HR	0.87	1.09
MAINTENANCE LABOR, 1.6%/YR OF BLI	1.16	1.07
CONTROL LAB LABOR, 20% OF OPERATING LABOR	<u>0.17</u>	<u>0.22</u>
LABOR COSTS	2.20	2.38
MAINTENANCE MATERIALS, 2.4%/YR OF BLI	1.16	1.07
OPERATING SUPPLIES, 10%/YR OF OPERATING LABOR	<u>0.09</u>	<u>0.11</u>
TOTAL DIRECT COSTS	97.59	92.43
PLANT OVERHEAD, 80% OF LABOR COSTS	1.76	1.90
TAXES AND INSURANCE, 2%/YR OF TFC	<u>1.34</u>	<u>1.08</u>
PLANT CASH COSTS	100.69	95.41
DEPRECIATION, 10%/YR OF TFC	<u>6.71</u>	<u>5.38</u>
PLANT GATE COSTS	107.40	100.79
G&A, SALES, RESEARCH	<u>12.00</u>	<u>15.00</u>
NET PRODUCTION COST	119.40	115.79
ROI BEFORE TAXES, 25%/YR OF TFC	<u>16.77</u>	<u>13.46</u>
PRODUCT VALUE	136.17	129.25

Economics for Nylon Resin SBUs

Table 2.6 summarizes the economics of SBUs for nylon 6 resins. Also listed in the table are economics for stand-alone nylon 6 resin plant under each of N6-SBU1 through N6-SBU4. In the case of N6-SBU5, two alternate cases, Case A and Case B, are presented. Similarly, those SBUs for nylon 66 resins are given in Table 2.7.

Among the N6-SBUs, N6-SBU4 provides the best economics both at the integrated plant and stand-alone nylon 6 resin plant. The economics for N6-SBU5 is less than desirable in both Case A and Case B. For the remaining three SBUs, their economics for the stand-alone nylon 6 plants are competitive within 6 % difference in product value. In the case of the integrated plant, the economics for N6-SBU2 is less favorable.

The economics for N66-SBU3 is less than desirable in both the integrated plant and the stand-alone nylon 66 resin plant. The size of the resin plant could be the major reason. The economics for the remaining for SBUs are competitive both at the integrated plant and the stand-alone plant with N66-SBU2 and N66-SBU4 more economically favorable.

Table 2.6
ECONOMICS OF SBUs FOR NYLON 6 RESINS

ECONOMIC COMPARISON

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

PEP COST INDEX: 624

	N6-SBU1	N6-SBU2	N6-SBU3	N6-SBU4	N6-SBU5 Case A
PRODUCTION CAPACITY, MILLION LB/YR (THOUSAND METRIC TON/YR)	154 (70)	154 (70)	187 (85)	154 (70)	165 (75)
INVESTMENT (\$ MILLIONS)					
BATTERY LIMITS (BLI)	200.2	244.4	222.4	210.1	152.2
OFFSITES	<u>131.7</u>	<u>151.4</u>	<u>131.4</u>	<u>129.9</u>	<u>185.2</u>
TOTAL FIXED CAPITAL (TFC)	331.9	395.8	353.8	340.0	337.4
PRODUCTION COSTS (\$/LB)					
RAW MATERIALS	31.31	31.83	43.56	11.86	40.73
BY-PRODUCTS	-3.46	-3.41	-3.28	--	--
UTILITIES	<u>17.42</u>	<u>19.95</u>	<u>12.87</u>	<u>19.06</u>	<u>25.28</u>
VARIABLE COSTS	45.27	48.37	53.15	30.92	66.01
LABOR COSTS	7.55	9.09	7.14	7.74	6.18
DIRECT COSTS	4.19	5.11	3.86	4.38	3.04
PLANT OVERHEAD, TAXES & INSURANCE	<u>10.34</u>	<u>12.40</u>	<u>9.49</u>	<u>10.60</u>	<u>9.02</u>
PLANT CASH COSTS	67.35	74.97	73.64	53.64	84.25
DEPRECIATION, 10%/YR OF TFC	<u>21.51</u>	<u>25.65</u>	<u>18.88</u>	<u>22.03</u>	<u>20.41</u>
PLANT GATE COSTS	88.86	100.62	92.52	75.67	104.66
G&A, SALES, RESEARCH	<u>12.00</u>	<u>12.00</u>	<u>12.00</u>	<u>12.00</u>	<u>12.00</u>
NET PRODUCTION COST	100.86	112.62	104.52	87.67	116.66
ROI BEFORE TAXES, 25%/YR OF TFC	<u>53.77</u>	<u>64.11</u>	<u>47.19</u>	<u>55.07</u>	<u>51.03</u>
PRODUCT VALUE	154.63	176.73	151.71	142.74	167.69

Table 2.6 (Concluded)
ECONOMICS OF SBUs FOR NYLON 6 RESINS

ECONOMIC COMPARISON

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

PEP COST INDEX: 624

ECONOMICS FOR STAND-ALONE NYLON 6 PLANT WITH CAPTIVE PRECURSOR

	N6-SBU1	N6-SBU2	N6-SBU3	N6-SBU4	N6-SBU5 Case B
INVESTMENT (\$ MILLIONS)					
BATTERY LIMITS (BLI)	56.2	56.2	62.5	56.2	248.9
OFFSITES	<u>41.5</u>	<u>41.5</u>	<u>46.9</u>	<u>41.5</u>	<u>315.0</u>
TOTAL FIXED CAPITAL (TFC)	97.7	97.7	109.4	97.7	563.8
PRODUCTION COSTS (¢/LB)					
RAW MATERIALS	72.22	79.61	81.13	64.26	76.98
BY-PRODUCTS	--	--	--	--	-110.00
UTILITIES	<u>4.39</u>	<u>4.39</u>	<u>4.39</u>	<u>4.39</u>	<u>46.18</u>
VARIABLE COSTS	76.61	84.00	85.52	68.65	13.16
LABOR & OTHER FIXED COSTS	<u>6.04</u>	<u>6.04</u>	<u>2.82</u>	<u>6.04</u>	<u>12.74</u>
PLANT CASH COSTS	82.65	90.04	88.34	74.69	39.07
PLANT GATE COSTS	88.98	96.37	96.76	81.02	73.18
NET PRODUCTION COSTS	100.98	108.37	108.76	93.02	85.18
PRODUCT VALUE	116.81	124.20	123.36	108.85	170.46

Table 2.7
ECONOMICS OF SBUs FOR NYLON 66 RESINS

ECONOMIC COMPARISON					
CAPACITY: 300 MILLION LB/YR (136,000 T/YR)					
PEP COST INDEX: 624					
	N66-SBU1	N66-SBU2	N66-SBU3	N66-SBU4	N66-SBU5 Case A
PRODUCTION CAPACITY, MILLION LB/YR (THOUSAND METRIC TON/YR)	176 (80)	176 (80)	99 (45)	209 (95)	298 (135)
INVESTMENT (\$ MILLIONS)					
BATTERY LIMITS (BLI)	222.4	219.4	181.0	195.4	260.4
OFFSITES	<u>113.3</u>	<u>111.6</u>	<u>89.6</u>	<u>101.8</u>	<u>233.7</u>
TOTAL FIXED CAPITAL (TFC)	335.7	331.0	270.5	297.2	494.1
PRODUCTION COSTS (\$/LB)					
RAW MATERIALS	34.94	30.45	32.05	34.94	41.86
BY-PRODUCTS	-1.83	-5.39	-2.87	-1.83	-0.08
UTILITIES	<u>9.51</u>	<u>9.51</u>	<u>11.21</u>	<u>7.77</u>	<u>17.59</u>
VARIABLE COSTS	42.62	34.57	40.39	40.88	59.37
LABOR COSTS	9.59	9.54	14.01	6.00	6.06
DIRECT COSTS	4.26	4.21	6.18	3.07	2.91
PLANT OVERHEAD, TAXES & INSURANCE	<u>11.48</u>	<u>11.38</u>	<u>16.66</u>	<u>7.64</u>	<u>8.17</u>
PLANT CASH COSTS	67.95	59.70	77.24	57.59	76.51
DEPRECIATION, 10%/YR OF TFC	<u>19.03</u>	<u>18.76</u>	<u>27.27</u>	<u>14.19</u>	<u>16.60</u>
PLANT GATE COSTS	86.98	78.46	104.51	71.78	93.11
G&A, SALES, RESEARCH	<u>15.00</u>	<u>15.00</u>	<u>15.00</u>	<u>15.00</u>	<u>15.00</u>
NET PRODUCTION COST	101.98	93.46	119.51	86.78	108.11
ROI BEFORE TAXES, 25%/YR OF TFC	<u>47.57</u>	<u>46.91</u>	<u>68.18</u>	<u>35.48</u>	<u>41.51</u>
PRODUCT VALUE	149.55	140.37	187.69	122.26	149.62

Table 2.7 (Concluded)
ECONOMICS OF SBUs FOR NYLON 66 RESINS

ECONOMIC COMPARISON

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

PEP COST INDEX: 624

ECONOMICS FOR STAND-ALONE NYLON 6 PLANT WITH CAPTIVE PRECURSORS

	N66-SBU1	N66-SBU2	N66-SBU3	N66-SBU4	N66-SBU5 Case B
INVESTMENT (\$ MILLIONS)					
BATTERY LIMITS (BLI)	55.6	55.6	40.7	61.2	356.5
OFFSITES	<u>28.6</u>	<u>28.6</u>	<u>20.3</u>	<u>31.5</u>	<u>365.8</u>
TOTAL FIXED CAPITAL (TFC)	84.2	84.2	61.0	92.7	722.3
PRODUCTION COSTS (\$/LB)					
RAW MATERIALS	62.86	60.34	79.56	58.73	62.22
BY-PRODUCTS	--	--	--	--	-90.15
UTILITIES	<u>1.88</u>	<u>1.88</u>	<u>1.89</u>	<u>1.88</u>	<u>29.20</u>
VARIABLE COSTS	64.74	62.22	81.45	60.61	1.27
LABOR & OTHER FIXED COSTS	<u>5.49</u>	<u>5.49</u>	<u>8.03</u>	<u>4.94</u>	<u>21.38</u>
PLANT CASH COSTS	70.23	67.71	89.48	65.55	22.65
PLANT GATE COSTS	75.00	72.48	95.63	69.98	46.92
NET PRODUCTION COSTS	90.00	87.48	110.63	81.98	61.92
PRODUCT VALUE	101.93	99.41	126.00	93.05	122.60

3 INDUSTRY STATUS

INTRODUCTION

Both nylon 6 and nylon 66 are consumed in the forms of resins and fibers. The United States, Western Europe and Japan are three major consumption regions with the United States consuming more nylon 66 than nylon 6 while Japan consuming more nylon 6 than nylon 66. In Western Europe the demand for nylon 6 is in par with that for nylon 66.

CONSUMPTION

Worldwide consumption of nylons in 2000 in the forms of resins and fibers is estimated to be about 6.2 million tons, of which approximately 60% is accounted for by nylon 66, and up to 40% by nylon 6. The remaining small percentage is for the other nylons, mainly nylon 46 and nylon 12. In fields of applications, about 75% of the total consumption is accounted for by fibers and the remainder by engineering plastics. The total year-2000 demand for nylon resins in the world major consuming regions, i.e. North America (the United States and Canada), Western Europe, portions of East Asia, was reported at 1.54 million metric tons. With present global economic slowdown, we estimated the total demand for nylon resins in these regions in 2005 at about 1.7 million tons, representing an average annual growth rate of 2%. The total demand for nylon fibers in the above major regions was estimated at about 3.56 million tons in 2000. The total demand in 2005 is estimated at 3.9 million tons. The major markets for nylon fibers are apparel, home furnishings, and industrial and consumer products.

Table 3.1 presents the distribution of nylon resins consumption in the United States in 2000. Those for the resins consumed in Western Europe and Japan are given in Tables 3.2 and 3.3, respectively. In the United States, the nylon resins are mostly consumed in injection molding, while extrusion accounts for more than 60% of the total nylon resin consumption in Japan, and 46% of the total consumption in Western Europe.

PRODUCTION CAPACITY

Producers of Nylon 6 Precursor

World producers for CAPM are given in Table 3.4 as of January 2000. The total production capacity is estimated at about 4.15 million ton/yr of which 31% is accounted for by the producers in Asia Pacific, 26% by the producers in Western Europe, 23% by the producers in North America, and the remainder by the producers in Eastern Europe. Except a few producers with their feedstocks unknown at the present time or using feedstocks, such as benzene, cyclohexanone and waste carpets, all other CAPM producers have their feedstocks based on either phenol or cyclohexane. About 20% of the total world CAPM production capacity is based on phenol, and 56% based on cyclohexane.

Table 3.5 shows the world large producers of CAPM with a total annual production capacity of 2.09 million metric tons, or 50% of the world total. BASF is the largest producer with a production capacity of 697,000 t/yr followed by DSM, AlliedSignal, China Petrochemical Development Corporation (CPDC), Ube Industries and Toray Industries. With the exception of the Allied Signal

plant, part of the plants of DSM and CPDC, all the other major producers use cyclohexane as a feedstock. Phenol is used in the Allied Signal plant at Hopewell, Virginia and the DSM plant at Geleen, the Netherlands. Benzene and cyclohexanone are used in two of CPDC plants.

Table 3.1
DISTRIBUTION OF NYLON RESINS
CONSUMPTION IN THE UNITED STATES

(THOUSANDS OF TONS PER YEAR)

	Nylon 66	Nylon6	Others
Injection Molding			
Automotive and Truck Parts	357	137	16
Electrical and Electronic Parts	78	11	9
Industrial Machinery Parts ^a	48	48	4
Consumer Articles	61	11	8
Hardware and Furniture Parts	15	7	—
Appliances Parts	15	10	1
Others	<u>15</u>	<u>8</u>	<u>—</u>
Injection Molding Total	589	252	38
Extrusion			
Film and Extrusion Coating ^a	14	100	6
Non-textile Monofilament ^a	12	15	18
Tubing and Pipe	6	19	23
Wire and Cable	—	70	4
Stock Shapes and Other	<u>15</u>	<u>9</u>	<u>8</u>
Extrusion Total	47	213	59
Total	636	465	97

^a Including additives, fillers and reinforcements; also reprocessed in others.

Source: Chemical Economics Handbook, SRI Consulting.

Table 3.2
DISTRIBUTION OF NYLON RESINS
CONSUMPTION IN WESTERN EUROPE

(THOUSANDS OF TONS PER YEAR)

	Nylon 66 &Nylon 6
Injection Molding	
Automotive and Truck Parts	175
Electrical and Electronic Parts	95
Appliances Parts	55
Others ^a	<u>95</u>
Injection Molding Total	420
Extrusion	
Films	67
Other ^b	<u>43</u>
Extrusion Total	110
Other Processing	10
Total	540

^a Including consumer, sports and recreation goods; also parts for building, furniture and machinery

^b Including shaped articles, such as sheets tube, cables and rods; also monofilaments

Source: Chemical Economics Handbook, SRI Consulting.

Table 3.3
DISTRIBUTION OF NYLON RESINS
CONSUMPTION IN JAPAN

(THOUSANDS OF TONS PER YEAR)

	Nylon 66	Nylon6	Others
Film and Sheet	—	40	—
Automotive and vehicle Parts	42	28	—
Electrical and Electronic Parts	17	20	—
Machinery Parts	7	8	—
Monofilament	—	4	—
Adhesives	—		1
Powder Coatings	—	—	0.5
Hoses and Tubing	—	—	5.5
Other	<u>8</u>	<u>16</u>	<u>15^a</u>
Total	74	116	22

^a Including mixed nylon films.

Source: Chemical Economics Handbook, SRI Consulting.

Table 3.4
WORLD PRODUCERS OF CAPROLACTAM
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Feedstock			Type of Process	Remarks			
		Phenol	Cyclohexane	Waste Carpet					
NORTH AMERICA									
United States									
AlliedSignal Inc.									
AlliedSignal Polymers									
Hopewell, VA	362.9	X			Allied Technology	Phenol is derived from purchased Cumene; most CAPM is captively consumed for production of nylon 6 fiber at Clemson, South Carolina, and resin at Chesterfield, Virginia and Columbia South Carolina.			
BASF Corp.									
Fiber Intermediate									
Freeport, TX	276.7		X		BASF Modified Nitric oxide Technology	CAPM is produced from purchased cyclohexane by modified nitric oxide process; most CAPM is captively consumed for nylon 6 fiber production at Clemson, South Carolina, Enka, North Carolina, and Lowland, Tennessee; and for nylon chips at Freeport, Texas.			
DSM Chemicals North America, Inc.									
Augusta, GA	195.0		X		DSM/HPO Process	Most CAPM for merchant, and some toll-converted for nylon chip also for merchant			
Evergreen Nylon Recycling LLC	45.4			X		Plant built under joint venture of AlliedSignal and DSM with each partner receiving half of the CAPM produced			
United States Total	880.0								
Mexico									
DuPont-Alpek									
Salamanca	75.0								
North America Total	955.0								
SOUTH AMERICA									
Brazil	55.0								
Columbia	30.0								
South America Total	85.0								
WESTERN EUROPE									
Belgium									
BASF Antwerpen N.V.									
Antwerpen	270.0		X		BASF Modified Nitric oxide Technology				
Bayer Antwerpen N.V.									
Antwerpen	135.0		X			Joint venture of DuPont and Rhone Poulenc, using DuPont's technology.			
Belgium Total	405.0								
Germany									
BASF Aktiengesellschaft									
Ludwigshafen	150.0		X			Plant restarted in 1992.			
DOMO Caproleuna GmbH									
Leuna	100.0	X							
Germany Total	250.0								
Italy									
EniChem Sri									
Porto Marghera	120.0	X							

Table 3.4 (Concluded)
WORLD PRODUCERS OF CAPROLACTAM
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Feedstock			Type of Process	Remarks			
		Phenol	Cyclohexane	Waste Carpet					
WESTERN EUROPE (concluded)									
Netherlands									
DSM Fibre Intermediates									
Geleen	220.0	X				The plant was acquired by Du Pont in 1992 from ICI, currently			
Spain									
Producto Quimicos del Mediterraneo, S.A.									
Castellon	75.0		X			Subsidiary of Ube Industries			
Western Europe Total	1070.0								
EASTERN EUROPE									
Bulgaria	24.0								
CIS	520.0								
Czech Republic	48.0								
Poland	137.0								
Romania	25.0								
Slovakia	28.0								
Eastern Europe Total	782.0								
ASIA PACIFIC									
China	115.0	X			DSM/HPO Process				
India	132.0	X							
Korea	120.0	X							
Japan									
EMS-UBE Ltd.									
Ube-shi, Yamaguchi Pref.	15.0	X				Almost all HMDA is captively consumed in the production of nylon 66 fibers, resins and HDI.			
Mitsubishi Chemical Corp.									
Kitakyushu, Fukuoka Pref.	110.0	X				Feed stock from waste caprolactam.			
Sumitomo Chemical Co. Ltd.									
Niihama, Ehime Pref.	80.0	X				15,000 t/yr expansion by 2005.			
Toray Industries, Inc.									
Nagoya, Aichi Pref.	85.0	X							
Tokai, Aichi Pref.	84.0	X							
Ube Industries, Ltd.									
Sakai, Osaka Pref.	110.0	X							
Ube, Yamaguchi Pref.	90.0	X							
Japan Total	574.0								
Taiwan	250.0	X			DSM/HPO Process	Feedstocks include benzene, cyclohexane and cyclohexanone			
Thailand	70.0	X							
Asia Pacific Total	1261.0								
WORLD TOTAL	4,153.0								

Sources: Chemical Economics Handbook, SRI Consulting and Trade literature

Table 3.5
WORLD SIX LARGEST PRODUCERS FOR CAPROLACTAM

PRODUCTION CAPACITY			
(THOUSANDS OF TONS PER YEAR)			
Companies	Capacity M t/yr	Location	Feedstock
BASF	277	Freeport, Texas, USA	Cyclohexane
	270	Antwerpen, Belgium	Cyclohexane
	150	Ludwigshafen, Germany	Cyclohexane
BASF Total	697		
DSM	195	Augusta, Georgia, USA	Cyclohexane
	220	Geleen, Netherlands	Phenol
	415		
AlliedSignal	363	Hopewell, Virginia, USA	Phenol
China Petrochemical Development Corp.	65	Toufen, miaoli Hsien, Taiwan	Benzene
	65	Kaohsiung, Taiwan	Cyclohexanone
	120	Shiaokang, Taiwan	Cyclohexane
CPDC Total	250		
Ube Industries	110	Sakai, Osaka Pref., Japan	Cyclohexane
	90	Ube, Yamaguchi Pref., Japan	Cyclohexane
	200		
Toray Industries	85	Nagoya, Aichi Pref., Japan	Cyclohexane
	84	Tokai, Aichi Pref., Japan	Cyclohexane
Toray Total	169		
Total	2094		

Source: Chemical Economics Handbook, SRI Consulting.

Producers of Nylon 66 Precursor

World producers for ADA and HMDA are given in Tables 3.6 and 3.7, respectively. The total production capacity for ADA is estimated at about 5.93 billion lb/yr (2.69 million ton/yr). The production capacity in North America accounts for 44% of the total, which is followed by 35% by the producers in Western Europe, 16% by the producers in Asia Pacific, and the remainder by the producers in Eastern Europe and South America. The total production capacity for HMDA is estimated at 3.42 billion lb/yr (1.55 million ton/yr), of which about 57% is located in North America and 33% in Western Europe. Feedstocks for HMDA production include butadiene at 46%, adiponitrile at 33%, and the remainder is acrylonitrile.

Table 3.8 gives the six large producers for both ADA and HMDA in the world. DuPont is the largest producer of both ADA and HMDA with production capacities of 1.23 million t/yr for ADA and 734,000 t/yr for HMDA at various locations worldwide. The follow-ups include Salutia, Rhodia, BASF and Asahi with a combined production capacity of the four at 1.12 million t/yr for ADA and 663,000 t/yr for HMDA. Overall, these major producers account for about 83% of total world capacity for ADA production, and 90% for HMDA production. As expected, most producers use cyclohexane as feedstock for ADA production except the plant of Asahi Chemical, which employs benzene as feedstock. For HMDA production, butadiene is used by most plants to prepare adiponitrile as an intermediate, which is hydrogenated to form HMDA. Alternatively, acrylonitrile is used by one BASF plant and one Salutia plant.

Producers of Nylon 6 and Nylon 66 Resins

World producers for nylon resins are listed in Table 3.9 with total production capacity of about 2.4 million metric tons of which about 31% is accounted for by nylon 66 resin production, 54% by nylon 6 resin production, and 15% by other nylons and unknown. The major production regions are Western Europe, North America and Asia Pacific with a distribution of about 44%, 24% and 23%, respectively in nylon 6 resin production, and a distribution of 44%, 29% and 22%, respectively in nylon 66 production.

Tables 3.10 present five large producers for nylon 66 resins with a total production capacity of 474,000 t/yr at about 64% of its total world production capacity. Table 3.11 gives six largest producers for nylon 6 resins with a total production capacity of 626,000 t/yr or about 48% of its total world production capacity.

Producers of Nylon 6 and Nylon 66 Fibers

The total world production capacity for both nylon 6 and nylon 66 fibers is reported at 5.4 million metric tons as of January 2000. Table 3.12 presents world six large nylon producers with a combined production capacity of 2.1 million t/yr, which accounts for about 39% of total world production capacity for nylon fibers. DuPont is the largest nylon producer with a worldwide production capacity of 911,000 t/yr or 17% of the world total. It is followed by Rhodia S.A. with a worldwide production capacity of 403,000 t/yr. The next four are Solutia, Formosa Plastics, BASF, and AlliedSignal. Specific breakdown of production capacity between nylon 6 and nylon 66 fibers is not available. However, based on the production capacity for nylon precursors that each of these major producers has, it appears that DuPont, Rhodia and Solutia are major nylon 66 producers whereas Formosa, BASF and AlliedSignal are major nylon 6 producers.

Table 3.6
WORLD PRODUCERS OF ADIPIC ACID
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Feedstock			Remarks		
		Phenol	Cyclohexane	Benzene			
NORTH AMERICA							
United States							
Du Pont Company							
Du Pont Chemicals							
Orange, TX	220.0		X		Purchased feedstock. Most adipic acid is captive for nylon 6,6 fiber and resins. Some goes to merchant.		
Victoria, TX	378.8		X				
Inolex Chemical							
Engineered Materials Sector							
Hopewell, VA	13.6	X			Adipic acid is a coproduct in the production of caprolactam. Sun Chemical acquired from AlliedSignal in mid-1998, and Inolex bought the unit in mid-1999. The majority of adipic acid is consumed for polyurethane production.		
Solutia							
Solutia							
Pensacola, FL	376.5		X		Purchased feedstock. Most adipic acid is captive for nylon 6,6 fiber and resins, and adipate plasticizers. Some goes to merchant.		
United States Total	988.8						
Canada							
Du Pont Canada							
Maitland, Ontario	190.0		X				
North America Total	1178.8						
WESTERN EUROPE							
Belgium							
UCB-Ftal sa							
Oostende	0.0		X		The plant is capable of producing adipic acid from phenol with production capacity reduced to 25,000 t/yr.		

Table 3.6 (Continued)
WORLD PRODUCERS OF ADIPIC ACID
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Feedstock			Remarks		
		Phenol	Cyclohexane	Benzene			
WESTERN EUROPE (concluded)							
France							
Rhodia Alsachimie SAS							
Chalampe	355.0		X		Plant capacity has been reported to be as low as 220,000 t/yr. Will build a \$100 million plant to become the largest producer in Europe		
Germany							
BASF Aktiengesellschaft							
Ludwigshafen	260.0		X				
Bayer AG							
Leverkusen	55.0		X				
Radici Chimica SpA							
Zeitz		X			Plant with 80,000 t/yr on stream in 2001.		
Germany Total	315.0						
Italy							
Radici Chimica SpA							
Novara	60.0	X			Plant purchased from Montedison and restarted in 1986. Plant capacity has been reported to be as high as 35,000 t/yr.		
United Kingdom							
Du Pont (UK) Ltd.							
Wilton	220.0		X		Plant's ownership has been transferred to Du Pont through swap agreement.		
Western Europe Total	950.0						
ASIA PACIFIC							
China							
CNP Liaoyang Petrochemical Fiber							
Liaoyang, Liaoning	100.0		X				
Pingdingshan Petrochemical							
Pingdingshan, Henan	37.0		X				
Taiyuan, Shanxi	2.0		X				
China Total	139.0						

Table 3.6 (Continued)
WORLD PRODUCERS OF ADIPIC ACID
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Feedstock			Remarks
		Phenol	Cyclohexane	Benzene	
ASIA PACIFIC (concluded)					
Japan					
Asahi Chemical Industry Co. Ltd.					
Nobeoka, Miyazaki Pref.	120.0			X	Self developed technology with purchased benzene
Kanto Denka Kogyo Co. Ltd.					
Shibukawa, Gunma Pref.			X		A 10,000 t/yr plant is on standby.
Sumitomo Chemical Co. Ltd.					
Niihama, Ehime Pref.	2.0		X		Adipic acid produced as a by-product of caprolactam production
Japan Total	122.0				
Korea, Republic of					
Kofran Chemical Co. Ltd.					
Ulsan, Kyongsangnam-do	65.0		X		
Singapore					
Du Pont Singapore					
Pulau Sakra	114.0		X		On stream 1994.
Taiwan					
Nan Ya Plastics					
Mailiao			X		A 40,000 t/yr plant to be on stream in 2002
Asia Pasific Total	440.0				
SOUTH AMERICA					
Brazil					
Rhodia S.A.					
Paulinia, Sao Paulo	67.0		X		

Table 3.6 (Concluded)
WORLD PRODUCERS OF ADIPIC ACID
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Feedstock			Remarks		
		Phenol	Cyclohexane	Benzene			
EASTERN EUROPE							
CIS (former USSR)							
State Complexes (2 Locations)	33.0						
Poland							
State Complexes (3 Locations)	18.0		X				
Romania							
State Complex	3.0						
Eastern Europe Total	54.0						
World Total	2689.8						

Sources: Chemical Economics Handbook, SRI Consulting, and Trade literature

Table 3.7
WORLD PRODUCERS OF HEXAMETHYLENEDIAMINE
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Feedstock			Remarks
		Butadiene	Acrylonitrile	Adiponitrile	
United States					
Du Pont de Nemours, E.I., and Co.					
Du Pont Chemical					
Orange, TX	331.1	X			Almost all HMDA is captively consumed in the production of nylon 6,6 fibers and resins. The remaining small quantities are sold on the merchant market. Plants use second-generation catalyst for hydrocyanation.
Victoria, TX	213.2	X			
Solutia Inc.					
Decatur, AL	136.1		X		Almost all HMDA is captively consumed in the production of nylon 6,6 fibers and resins. The remaining small quantities are sold on the merchant market.
Pensacola, FL	129.3		X		
United States Total	810.0				The unit was shut down in 1980, but now continues to produce HMDA with adiponitrile from imports or from Decatur.
Canada					
Du Pont Canada, Inc.					
Maitland, Ontario	70.0		X		Adiponitrile imported from Du Pont's U.S. plant.
North America Total	880.0				
SOUTH AMERICA					
Brazil					
Rhodia (Brazil)					
Paulinia, Sao Paulo	33.0				
WESTERN EUROPE					
France					
Rhodia S.A.					
Saint Fons	110.0		X		
SNC Butachimie					
Chalampe	130.0	X			Joint venture of Du Pont and Rhodia, using Du Pont's technology. The ADN capacity in this location was expanded to 500,000 t/yr
France Total	240.0				
Italy					
Radici Chimica SpA					
Novara	30.0		X		Plant restarted in 1992.
United Kingdom					
BASF plc					
Middlebrough	115.0	X			
Du Pont (UK) Ltd.					
Wilson	120.0		X		The plant was acquired by Du Pont in 1992 from ICI, currently operating on imported ADN. The original 110,000 t/yr ADN plant (owned by ICI) was shut down.
United Kingdom Total	235.0				
WESTERN EUROPE TOTAL	505.0				

Table 3.7 (Concluded)
WORLD PRODUCERS OF HEXAMETHYLENEDIAMINE
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Feedstock			Remarks
		Butadiene	Acrylonitrile	Adiponitrile	
EASTERN EUROPE					
Russia					
State Complexes					
2 locations	11.0				Plants reportedly not operating.
Ukraine					
State Complexes					
2 locations	20.0				
ASIA PACIFIC					
China					
Liaoyang Petrochemical Fiber					
Liaoyang, Liaoning	22.0			X	Plant currently uses Rhone Poulenc technology.
Pindingshan Nylon Cord Fabrics Plant					
Pingdingshan, Henan	29.5			X	Plant using Asahi Chemical process technology has production capacity of 65,000 t/yr. It was on stream 1997.
China Total	51.5				
Japan					
Asahi Chemical Industry Co., Ltd.					
Nobeoka, Miyazaki Pref.	43.0	X			Almost all HMDA is captively consumed in the production of nylon 66 fibers, resins and HDI.
Toray Industries, Inc.					
Nagoya, Aichi Pref.	2.0				Feed stock from waste caprolactam.
Japan Total	45.0				
ASIA TOTAL	96.5				
WORLD TOTAL	#####				

Sources: Chemical Economics Handbook, SRI Consulting and Trade literature

Table 3.8
WORLD FIVE LARGEST PRODUCERS
FOR ADIPIC ACID and HEXAMETHYLENEDIAMINE

Companies	PRODUCTION CAPACITY		Location	Feedstock
	ADA Capacity M t/yr	HDMA Capacity M t/yr		
DuPont	220	331	Orange, Texas, USA	Cyclohexane and butadiene
	379	213	Victoria, Texas, USA	
	190	70	Maitland, Ontario, Canada	
	220	120	Wilton, United Kingdom	
	114		Pulau Sakra, Singapore	
DuPont Total	1123	734		
Salutia	377	129	Pensacola, Florida, USA	Cyclohexane and adiponitrile
		136	Decatur, Alabama, USA	Acrylonitrile
Salutia Total	377	265		
Rhodia Alsachimie	355	130	Chalampe, France	Cyclohexane and butadiene
		110	Saint Fons, France	
Rhodia Total	355	240		
BASF	260	115	Ludwigshafen, Germany	Cyclohexane
			Middlebrough, United Kingdom	Acrylonitrile
BASF Total	260	115		
Asahi Chemicals	120	43	Nobeoka, Miyazaki Pref., Japan	Benzene and butadiene
Asahi Total	120	43		
Total	2235	1397		

Source: Chemical Economics Handbook, SRI Consulting.

Table 3.9
WORLD MAJOR PRODUCERS OF NYLON RESINS
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Resins			Remarks		
		Nylon 6	Nylon 66	Other nylons			
NORTH AMERICA							
United States							
BASF Corp.							
Plastic Materials Group, Polymers Division							
Hopewell, VA	61.0	X			Ultramid® nylon 6 with captive CAPM		
Custom Resins Inc.							
Hendersonville, NC	14.0				Nylene®, also making copolymer nylons		
DSM Chemicals North America, Inc.							
Augusta, GA	15.0	X					
DuPont							
DuPont Engineering Polymers, DuPont Polymers							
Chattanooga, TN	25.0		X	X	Zytel®HTN		
Parkersburg, WV	159.0	X	X	X	Zytel®66 and Zytel®612; Minlon® and Selar®		
Honeywell					Company purchased and its name adopted by AlliedSignal in 1999		
Chesterfield, VA	102.0	X			Capron®		
Columbia, SC	34.0	X					
Nyltec North America					Owned jointly by Rhodia and Caffaro SpA		
Manchester, NH	12	X					
Solutia					Company spun off from Monsanto in September 1997		
Chemical Group							
Pensacola, FL	95		X	X			
Ticona LLC					Company spun off from Hoechst Celanese		
Bishop, TX	40		X				
United States Total	557.0						

Table 3.9 (Continued)
WORLD MAJOR PRODUCERS OF NYLON RESINS
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Resins			Remarks		
		Nylon 6	Nylon 66	Other nylons			
SOUTH AMERICA							
Argentina							
DuPont Argentina S.A.							
Beraztequi	10		X				
SNIFA S.A.I.C.F.el.							
Jose Hernandez	1		X				
Argentina Total	11						
Brazil							
De Millus S/A Industriae Comercio							
Rio de Janeiro	1	X					
SOUTH AMERICA (concluded)							
Brazil (concluded)							
Mazzaferro Tecnopolimeros Ltda.							
Sao Bernardo do Campo	7	X					
Petrony Industria e Comercio de Poliamida Ltda.							
Embu	4	X	X				
Rhodia S.A.							
Santo Andre	11		X				
Sao Bernado do Campo	7		X				
Brazil Total	30						
South America Total	41						
WESTERN EUROPE							
Belgium							
BASF Antwerpen N.V.							
Antwerpen	60	X			Ultramid®		
DuPont de Nemours (Belgium)							
Mechelen	50	X			Zytel®		
Belgium Total	110						
France							
ATOFINA					The chemical branch of TotalFinaElf		
Serquigny	33	X		X	Rilsan®		
Rhodia Engineering Plastic S.A.							
Saint Fons	90	X	X		Technyl®		
France Total	123						

Table 3.9 (Continued)
WORLD MAJOR PRODUCERS OF NYLON RESINS
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Resins			Remarks
		Nylon 6	Nylon 66	Other nylons	
Germany					
ATOFINA Deutschland GmbH					
Bonn	5	X	X		Copolyamide of nylon 6,66, and 12 Platamide® and Platilon®
BASF Aktiengesellschaft					
Ludwigshafen	40		X		Ultramid®A
	70	X			Ultramid®B
Bayer AG					
Krefeld	100	X	X		Durethan®
Degussa AG					
Marl	14			X	Vestamid® and Vestoint®, nylon 12 and 612
Witten	5	X			Trogamid®Copolymers
DSM Deutschland GmbH					
Obernburg am Main	13		X		Akulon®
DuPont de Nemours (Deutschland) GmbH					
Hamm-Uentrop	60		X		Zytel®
Honeywell Polymers GmbH					
Rudolstadt	30	X	X		Resin and Compounding, Capron® and Nypel®
Leuna-Miramid GmbH					
Leuna	10	X	X		Miramid®
PLASTOMID Polymere GmbH					
Guben	20	X			Ponamid®
Solvay Advanced Polymers GmbH					
Rheinberg	5			X	Polyarylamide, partially aromatic nylon; IXef®
Germany Total	372				
Italy					
Aquafl SpA					
Arco	8	X			
Caffaro Flexible Packaging SpA					
Ceriano-Laghetto	35	X			Nylon 6 for films
Radicifil Srl, Textile Produkte SpA					
Radici Chimica SpA					
Casnigo, Gandino, Novara	40	X	X		Radilon®
Rhodia Engineering Plastics S.r.l.					
Ceriano-Laghetto	20		X		Technyl®
	10	X			
Italy Total	113				

Table 3.9 (Continued)
WORLD MAJOR PRODUCERS OF NYLON RESINS
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Resins			Remarks
		Nylon 6	Nylon 66	Other nylons	
Netherlands					
DSM Engineering Plastics					
Emmen	85	X			Akulon®
Geleen	20			X	Stanyl®
DuPont Dow Elastomers BV					
Rozenburg	20	X	X		Maranyl®
Netherlands Total	125				
Spain					
Polibasa					
Barbastro	8	X	X		Bergamid®
Poliseda					
Alcala de Henares	23	X			Arion®
Spain Total	31				
Switzerland					
EMS-CHEMIE AG					
Domat Ems	40	X	X	X	Grilon®, Griamid®
United Kingdom					
DuPont (U.K.) Ltd.					
Wilton	20		X		
Western Europe Total	934				
CENTRAL EUROPE					
Czech Republic					
SPOLANA a.s.					
Neratovice	1	X			May be only compounding.
Hungary					
Zoltek Vegyipari Rt.					Owned by Zoltek, USA
Nyergesujfalu	3	X			
Poland					
Polimix-Cekop a.s.					
Warszawa	na	X			
Stilon					
Gorzow	10	X		X	Owned 75% by Rhodia S.A.; Technyl®
Zaklady Azotowe w Tarnowie-Moscicach, S.A.					
Tarnow	23	X			Tarnamide®
Slovakia					
Povazske Chemicke Zavody, a.s.					
Zilina	4	X			
Central Europe Total	41				

Table 3.9 (Continued)
WORLD MAJOR PRODUCERS OF NYLON RESINS
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Resins			Remarks
		Nylon 6	Nylon 66	Other nylons	
EASTERN EUROPE					
Belarus	30	X			
Georgia	30	X			
Russia	250				Estimated
Ukraine	18	X	X		Some capacity not available
Eastern Europe Total	328				
Central & Eastern Europe Total	369				
ASIA PACIFIC					
China			X		
Korea					
AlliedSignal Co. Ltd.					
Iri, Chollabuk-do	6	X			
Hyosung Corp.					
Anyang, Kyonggi-do	23	X	X		
Kolon Industries, Inc.					
Kumi, Kyongsangbuk-do	14	X	X		Kopa®
Korea Total	43				
Japan					
Asahi Chemical Industry Co. Ltd.					
Nobeoka, Miyazaki Pref.	45		X		
Mitsubishi Engineering Plastics Corp.					
Kurosaki, Fukuoka Pref.	30	X			Joint Venture of Mitsubishi Gas Chemical and Mitsubishi Kasei
Mitsubishi Gas Chemical Co. Inc.					
Niigata, Niigata Pref.	15				
Mitsui Chemicals, Inc.					
Kuga-gun, Yamaguchi Pref.	3.2				Product of HMDA and terephthalic acid
Toray Industries, Inc.					
Nagoya, Aichi Pref.	28	X			
	22		X		
	2.9			X	
Toyobo Co. Ltd.					
Tsuruga, Fukui Pref.	15	X			

Table 3.9 (Concluded)
WORLD MAJOR PRODUCERS OF NYLON RESINS
AS OF JANUARY 2000

Company and Plant location	Capacity (1,000 t/yr)	Type of Resins			Remarks		
		Nylon 6	Nylon 66	Other nylons			
ASIA PACIFIC (concluded)							
Japan (concluded)							
Ube Industries, Ltd.							
Ube, Yamaguchi Pref.	55	X					
	7		X				
	6.5			X			
Unitika Ltd.							
Uji, Kyoto Pref.	34	X					
Japan Total	263.6						
Singapore							
DuPont Singapore Pte. Ltd.							
Jurong Island	60		X				
Taiwan							
China Petrochemical Development Corp.							
Toufen, Miaoli Hsien	70	X					
Ginar Chemical Co. Ltd.							
Tayuan Hsiang, Taoyuan Hsien	10	X	X				
Nyltech Taiwan Co. Ltd.							
Tunglo Hsiang, Miaoli Hsien	6		X				
Tai Young Nylon Co. Ltd.							
Taliao Hsiang, Kaohsiung Hsien	11	X					
Taiwan Total	97						
Thailand							
Ube Nylon Co. Ltd.							
Rayong, Rayong	15	X					
Asia Pacific Total	478.6						
World Total	2379.6						

Table 3.10
WORLD LARGEST PRODUCERS FOR NYLON 66 RESINS

PRODUCTION CAPACITY		
(THOUSANDS OF TONS PER YEAR)		
Companies	Capacity M t/yr	Location
DuPont	79	Parkersburg, West Virginia, USA
	25	Chattanooga, Tennessee, USA
	60	Hamm-Uentrop, Germany
	20	Wilton, United Kingdom
	10	Rozenburg, the Netherlands
	10	Beraztequi, Argentina
DuPont Total	204	
Salutia	95	Pensacola, Florida, USA
Bayer	50	Krefeld, Germany
Asahi Chemicals	45	Nobeoka, Miyazaki Pref., Japan
BASF	40	Ludwigshafen, Germany
Total	474	

Source: Chemical Economics Handbook, SRI Consulting.

Table 3.11
WORLD LARGEST PRODUCERS FOR NYLON 6 RESINS

PRODUCTION CAPACITY		
Companies	Capacity M t/yr	Location
BASF	61	Hopewell, Virginia, USA
	70	Ludwigshafen, Germany
	60	Antwerpen, Belgium
BASF Total	191	
Honeywell	102	Chesterfield, Virginia, USA
	34	Columbia, South Carolina, USA
	15	Rudolstadt, Germany
Honeywell Total	151	
DuPont	79	Parkersburg, West Virginia, USA
	50	Mechelen, Belgium
	10	Rozenburg, the Netherlands
DuPont Total	139	
DSM	85	Emmen, the Netherlands
	15	Augusta, Georgia, USA
DSM Total	100	
Solutia	95	Pensacola, Florida, USA
China Petrochemical Development Corp.	70	Toufen, Miaoli Hsien, Taiwan
Total	626	

Source: Chemical Economics Handbook, SRI Consulting.

Table 3.12
WORLD LARGEST PRODUCERS FOR NYLON FIBERS

PRODUCTION CAPACITY		
(THOUSANDS OF TONS PER YEAR)		
Companies	Capacity M t/yr	Location
DuPont	504	United States
	160	Germany
	90	Canada
	35	United Kingdom
	122	Other countries
DuPont Total	911	
Rhodia S.A.	74	United States
	64	Poland
	54	France
	51	Italy
	50	Brazil
	110	Other countries
Rhodia Total	403	
Solutia Inc.	336	United States
Formosa Plastics	229	Taiwan
BASF	138	United States
AlliedSignal	94	United States
Total	2111	

Source: Chemical Economics Handbook, SRI Consulting.

4 REVIEW OF TECHNOLOGY FOR NYLONS AND THEIR PRECURSORS

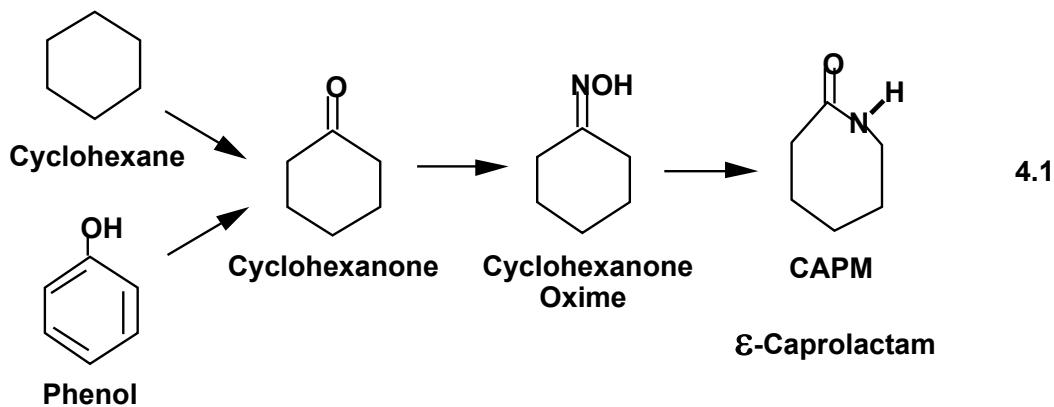
In this report, we review recent technology developments in processes for the production of precursors for nylon 6 and nylon 66; they are ϵ -caprolactam (CAPM), hexamethylene diamine (HMDA) and adipic acid (ADA). Also reviewed are technology in processes for the production of respective nylon 6 and nylon 66. All the patents reviewed in this section are assigned to major companies for the past five years, and summarized in tables given in Appendix A of this report.

REVIEW OF TECHNOLOGY FOR NYLON 6 AND ITS PRECURSOR

Table 4.1 presents an annotated list of patents for technology for preparation of CAPM, while Tables 4.2 and 4.3 summarize the patents for nylon 6 by hydrolytic polymerization and anionic polymerization, respectively.

Technology for Caprolactam

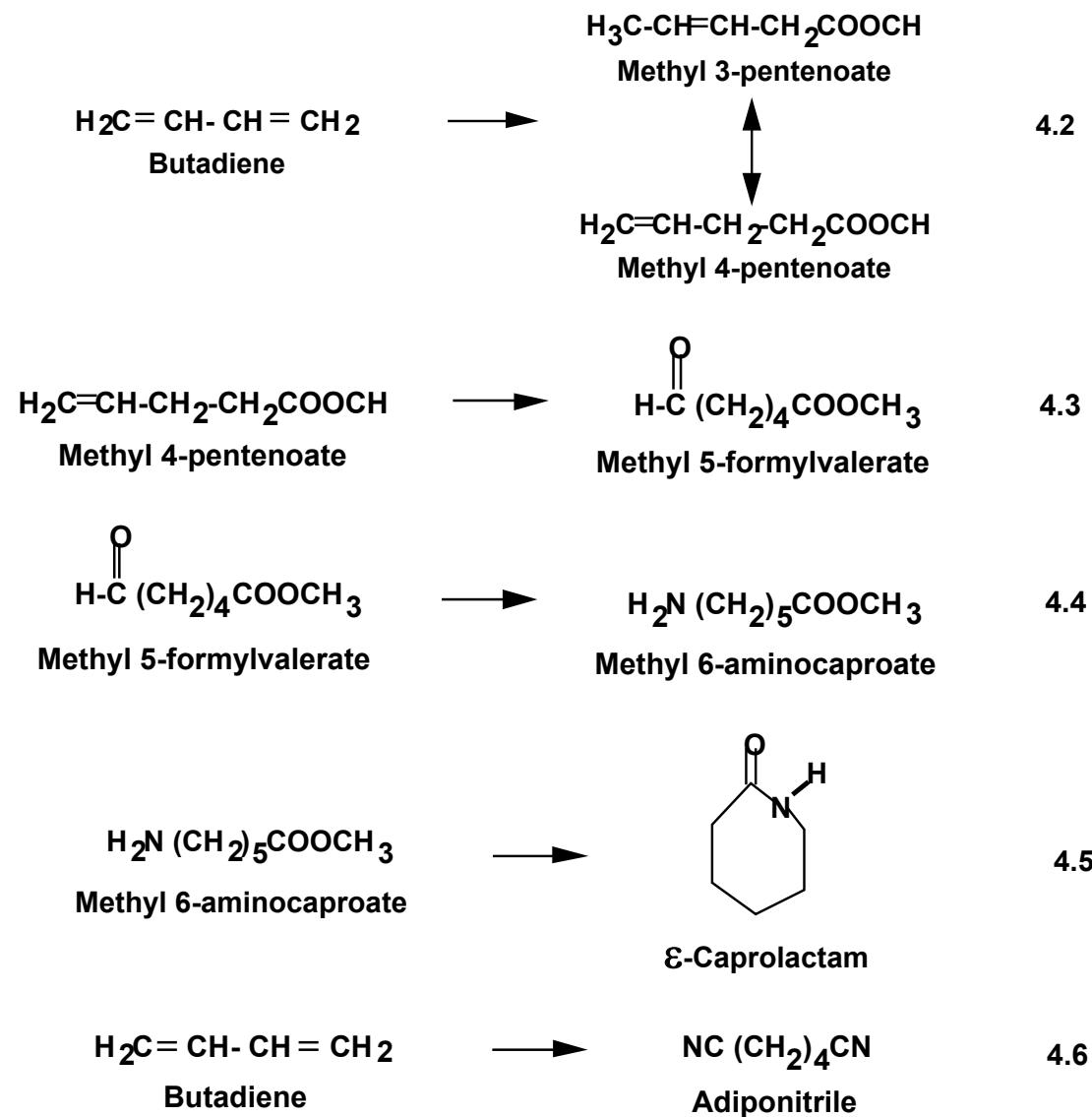
At the present time, most of CAPM plants use cyclohexane as a starting raw material to prepare cyclohexanone, a precursor of CAPM with exceptions that use phenol in stead of cyclohexane. They are AlliedSignal Polymers in the United States, and DSM and EniChem in Western Europe. Cyclohexanone is prepared either by oxidation of cyclohexane or hydrogenation of phenol. It is then converted to cyclohexanone oxime, which is further converted to CAPM through Beckmann rearrangement as indicated in reaction 4.1.

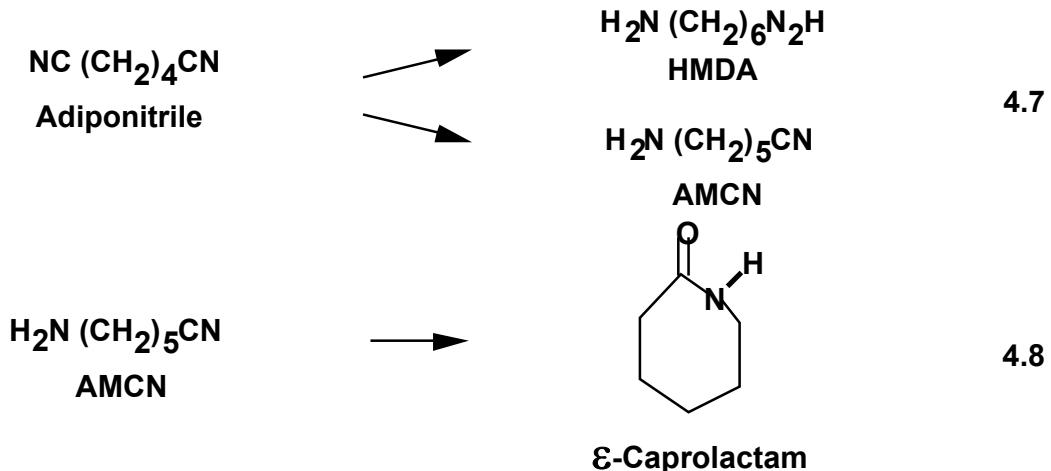


Since mid 1990s, several new routes have been developed to produce CAPM from butadiene. The following two processes have recently been commercialized:

- DSM-DuPont technology – Butadiene is carbonylated to methyl pentenoate followed by hydroformylation to methyl formylvalerate. The latter is subjected to reductive ammoniation to methyl 6-aminocaproate, which is then cyclized to CAPM.
- BASF-DuPont technology – Butadiene is converted to adiponitrile (ADN) in two-step hydrocyanation. ADN is then partial hydrogenated to HMDA and 6-aminocapronitrile. The latter is then cyclized to CAPM.

The major operations for the above two processes are shown in reaction 4.2 through 4.5 and 4.6 through 4.8, respectively.





Preparation of Cyclohexanone

Cyclohexanone is prepared from either phenol by hydrogenation or cyclohexane by oxidation. Patents pertaining to the technology for the preparation of cyclohexanone from phenol or cyclohexane are mostly reviewed in PEP Report 41B (March 1988) and PEP Report 7C (May 1998). Only a few patents are listed in Table 4.1 in the present report.

It is well known that phenol is hydrogenated over nickel catalysts to give predominately cyclohexanol, or hydrogenated over noble metal catalysts, such as Pd, Rh or Pt, to give mostly cyclohexanone. In CA 2285828, phenol is reportedly hydrogenated in liquid phase at 140°C and 0.5 MPa in the presence of Pd catalyst supported on active carbon and promoted with sodium formate. The conversion is reported near complete and the selectivity to cyclohexanone is 94.5%. The catalyst is prepared from aqueous solutions of tetrachloropalladic acid and sodium formate. The pH of the solutions is kept at 6 to achieve a catalyst with high activity. In US 5395976, Pd catalyst supported on Li-Al spinel is prepared from sodium palladium chloride (Na₂PdCl₄) by reduction with hydrazine. After washing and drying, the catalyst is activated with a mixture of 10 vol% hydrogen and 90 vol% nitrogen at 350-400°C for 24 hours. The catalyst is used for gas-phase hydrogenation at 150°C with a molar ratio of hydrogen to phenol at 4:1. The conversion of phenol is > 97% with selectivity to KA oil (a mixture of cyclohexanone and cyclohexanol) at > 99.9%. The molar ratio of cyclohexanone to cyclohexanol, or KA ratio, reported at 47:1 initially and 16-18:1 after more than 2500 hours. The catalyst is regenerated with air at 350-500°C for 4-16 hours. After displacing the air with nitrogen, the catalyst is reduced with a mixture of 10 vol% hydrogen and 90 vol% nitrogen at 150°C for 4 hours.

An alternative route for cyclohexanone production is cited in US 5900482. In the process, cyclohexene is hydrated to cyclohexanol at 120°C under nitrogen in the presence of gallium catalyst supported on silica. Cyclohexanol is then dehydrogenated to cyclohexanone at 250°C a copper oxide-chromium oxide catalyst. The yield for both reactions is low.

Preparation of Cyclohexanone Oxime

Cyclohexanone oxime is prepared from cyclohexanone by ammoximation. Commercially, there are mainly three processes used in the industry. They are the HPO process using hydroxylammonium phosphoric acid as a carrier of hydroxylamine, the catalytic nitric oxide

reduction process using hydroxylammonium sulfate as a hydroxylamine carrier, and the Raschig process also using hydroxylammonium sulfate as a hydroxylamine carrier.

In early 1990s, Enichem has developed a new process for producing cyclohexanone oxime without using technology with hydroxylammonium phosphoric acid or hydroxylammonium sulfate (US 5312987, US 5227525). The process involves direct reaction of cyclohexanone with ammonia and hydrogen peroxide over a Ti-silicate catalyst without emission of NO_x or SO_x. In the process, cyclohexanone in t-butanol reacts with excess ammonia and 49.7 wt% aqueous hydrogen peroxide at 85°C for about 1.2 hours in the presence of suspended Ti catalyst. The use of t—butanol is to promote the reaction by solubilizing cyclohexanone in the aqueous hydrogen peroxide. The conversion of cyclohexanone is 98.3% with 99.6% selectivity to oxime. The resulting mixture is further reacted with a hydroxylamine solution at 85°C for about 30 min to convert the residual cyclohexanone to oxime. Similar process is also cited in US 5599987 and US 5451701. In that process, a facility for making hydrogen peroxide from isopropanol by oxidation is also incorporated. Acetone formed during the oxidation is separated from the hydrogen peroxide along with unreacted isopropanol. The acetone is hydrogenated later to regenerated isopropanol.

In US 5684201, cyclohexanone reacts with excess ammonia at 80°C in a fixed bed reactor packed with either TiO₂ or γ -alumina to form cyclohexylideneamine (cyclohexanoneimine) and water. The reaction mixture is mixed with chlorobenzene, and the resulting mixture is distilled to remove excess ammonia, and the resulting mixture is decanted to separate the aqueous layer. The cyclohexylideneamine in chlorobenzene is subjected to oxidation at 100°C with air in the presence of Ti(BuO)₄ (1 g catalyst per 10 g cyclohexylideneamine) to produce cyclohexanoneoxime. In both steps, the conversion is complete. The selectivity to cyclohexylideneamine in the first step is 92-95%, but the selectivity to cyclohexanone oxime in the second step is low at 46%.

Beckmann Rearrangement of Cyclohexanone Oxime

Beckmann rearrangement is carried out in either liquid phase or gas phase. In the former case, the reaction takes place at a temperature of 85-125°C in the presence of oleum, while in the latter case the reaction occurs at about 300°C or higher in the presence of a heterogeneous catalyst. The liquid-phase rearrangement is widely employed in the industry. However, the process consumes significant amounts of sulfuric acid, and typically generates 1.7 tons of ammonium sulfate for every ton of CAPM produced. It is desirable to keep acid consumption as small as possible in order to minimize the production of ammonium sulfate. However, as the ratio of oleum to oxime decreases there is possibility of producing CAPM with less desirable quality, i.e. the formation of octahydrophenazine (C₆H₈N₂C₆H₈), which is UV active compound undesirable for high purity CAPM for nylon 6 production (US 6252068). For a CAPM producer, having difficulties to sell or dispose the sulfate by-product, the gas-phase Beckmann rearrangement is a preferable alternative. Otherwise, the liquid-phase Beckmann rearrangement is still logical choice.

CAPM with improved purity is produced in a liquid-phase rearrangement process cited in US 5264571. In the process, cyclohexanone oxime is completely converted in two to three reactors in series. In the operation, more than 60% of the oxime and all oleum are added to the first reactor. The remaining oxime is added in decreasing amount to the following reactors. The improvement is to recycle about 20 vol% of the reactor effluent from the last stage to the previous stage. Overall, the conversion of the oxime is complete with a selectivity of >99% to CAPM.

Zeolite catalyst is used for the gas-phase Beckmann rearrangement, which can be operated either in a fixed-bed reactor or fluid-bed reactor. The catalyst is extruded to particles with sizes of

0.5-5 mm for fixed-bed process, while with sizes of 80-250 µm for fluid-bed process. A boron-containing pentasil zeolite catalyst is reportedly employed for the gas-phase Beckmann rearrangement in fixed-bed reactor at 300°C and 0.01 MPa (US 6071844, US 6051706, US 5741904), providing a conversion of 96-97% and a selectivity of 92-97%. In the operation, cyclohexanone oxime is dissolved in ethanol (ethanol/oxime 9:1 by weight) and any additive components, and then evaporated and fed along with a carrier gas into a fixed-bed reactor packed with the boron-containing pentasil zeolite catalyst. The weight hourly space velocity (WHSV) is reported at 0.25-0.33 hr⁻¹. The catalyst is regenerated with air or oxygen at 450-500°C for more than 16 hours.

In US 6265574 B1 and US 6258949 B1, a fluid-bed reactor is used for the gas-phase Beckmann rearrangement with a similar zeolite catalyst described above. A separate fluid-bed regenerator is attached to the main reactor so that a part of the catalyst is continuously or intermittently withdrawn from the main reactor and fed to the regenerator through a control valve. The regenerated catalyst is withdrawn from the fluid-bed regenerator, and recycled to the main reactor through a screw feeder. Nitrogen is used to carry the regenerated catalyst.

Caprolactam from Butadiene

CAPM can be prepared by cyclization of 6-aminocapronitrile (6AMCN), methyl 6-amino-caproate (M6AMC), 6-aminocaproic acid (6AMCA) or 6-aminocaproic amide (6ACAM). The first precursor is derived from butadiene by hydrocyanation while the last three are derived from butadiene by hydrocarboxylation.

CAPM Precursors from Butadiene by Hydrocyanation

Butadiene is hydrocyanated to adiponitrile (ADN), which is up to now mostly used as a precursor for hexamethylene diamine (HMDA). Typically, the hydrocyanation is carried out in the presence of nickel and a phosphorus-containing ligand. A list of patents pertaining to this technology is presented in Table 4.5 of this report, and a review of this technology will be presented later in this section. As mentioned earlier, a technology to produce both 6AMCN and HMDA by partial hydrogenation of ADN has been developed since mid 1990s. A list of patents pertaining to this technology is given in Table 4.1.

Partial Hydrogenation of Adiponitrile

6AMCN is prepared along with HMDA by partial hydrogenation of ADN. Various catalyst systems have been reported for this purpose. Raney nickel and Raney cobalt are major components in those systems with a promoter selected from metals, such as palladium, platinum, silver, iron, chromium or tungsten (US 6147247, US 6147208, US 6114567, US 6110856, US 6080883, US 5874607, US 5801268, US 5801267, US 5789621, US 5756808). A base, such as alkali metal hydroxides or ammonium hydroxide can also be used to promote the yield of AMCN (US 5717090). ADN prepared from the hydrocyanation has a phosphorus content of about < 50 ppm. The phosphorus is preferably reduced to < 1 ppm by extraction with caustic soda solution, by adsorption with calcium oxide, or by distillation (US 6147247).

The partial hydrogenation can be carried out in a fixed-bed reactor by trickel-bed liquid phase manner or in an autoclave with suspension catalysts. The reaction temperature ranges from 50 to 120°C and reaction pressure from 4 to 20 MPa, depending on the type of catalyst used and desired conversions and selectivities. The molar ratio of 6AMCN to HMDA can be controlled by the conversion of ADN chosen. In general, a conversion of 30-80 is preferred for a

relatively higher selectivity to 6AMCN than that to HMDA (US 7147247). The selectivity increases as the conversion decreases (US 6080883).

The reaction products from the partial hydrogenation comprise 6AMCN, HMDA, unreacted ADN and tetrahydroazepine (THA, C₆H₁₁N). THA, which is about 1000 ppm based on HMDA, is difficult to be separated from the reaction products, 6AMCN in particular.

Alternatively, 6AMCN can be prepared from 5-formylvaleronitrile (5FVN) by reductive ammoniation (US 6048997, US 6121481) in the presence of a hydrogenation catalyst selected from metals, such as Ru, Co, and Pd supported on alumina. The ammoniation reaction takes place at 80-100°C, and conversion is complete after > 20 hours with a selectivity of 56-73% to AMCN, or 62-85% to AMCN and HMDA. The by-products are valeronitrile, 3- and 4-formylvaleronitriles, and 6-hydroxycapronitrile. In this case, the 5FVN is prepared by hydroformylation of pentenenitrile, an intermediate in the hydrocyanation of butadiene.

Cyclization of 6AMCN

AMCN is cyclized to form CAPM by reacting AMCN with water in the presence of catalysts in either gas-phase or liquid-phase reaction. In the earlier patents, the reaction took place in gas-phase at 300°C in the presence of solid catalysts, such as acidic silica gel or oxides of Cu, Cr, Ba, and Ti. These catalysts provide good initial conversion and selectivity to CAPM, but their activity declines rapidly during the reaction (US 5739324). In US 5493021, a phosphate salt of lanthanum or aluminum is used as a heterogeneous catalyst for the gas-phase reaction in a fixed-bed reactor. The reaction takes place at 280-300°C. The conversion is reported at 69% and selectivity at 97% with LaPO₄ catalyst doped with cesium hydrogenphosphate. The activity of this catalyst is 0.63 g CAPM per ml of catalyst per hr, and it has a longer live than the other catalysts, such as LaPO₄ without doping and LaPO₄ calcined at 700°C.

Liquid-phase cyclization reaction can be carried out with or without a catalyst. In the former case, titanium oxide extrudates are used to pack in a fixed-bed reactor. The reaction takes place at 180-240°C with a conversion of 6AMCN at 98% and a selectivity of 92% for a residence time of 0.25 hour (US 5874575, US 5739324, US 5693793, US 5495014). The conversion is complete when the residence time reaches to 0.5 hour or longer, but the selectivity drops to 76-88%. In the latter case, an aqueous solution of 6AMCN is heated at 300°C for 1 hour to obtain a mixture of 76 wt% CAPM and a remainder of oligomers (US 5495016).

The cyclization of AMCN with water forms CAPM and ammonia along with some oligomers, which have end groups, such as carboxyl, carbamoyl, nitrile, and/or, ester when alcohols are used as a solvent for the reaction. These high boilers have to be removed from CAPM because they are different from Nylon 6 formed from the ring-opening polycondensation in two aspects – (1) they have relatively low MW with broad distribution, and (2) they have various end groups other than the carboxyl groups in the chemistry structure.

CAPM Precursors from Butadiene by Hydrocarboxylation

As mentioned earlier, M6AMC is the major intermediate in the process developed jointly by DSM and DuPont. Initially, methyl pentenoats or their corresponding acids are prepared by hydrocarboxylation of butadiene with or without methanol as shown in reaction 4.2. A list of patents pertaining to this reaction will be reviewed later under technology for making adipic acid from butadiene. In the meantime, US 6175036 cites a route to prepare methyl pentenoats by converting butadiene first to 3-methoxy-1-butene in the reaction of methanol in toluene with butadiene in the presence of acidic ion exchanger at 120°C under nitrogen. The 3-methoxy-1-butene is then carbonylated to 3-methoxy-1-butene at 140°C and 5 MPa in the presence of Pd-

acetate and a promoter, such as bis(diphenylphosphino)butane, 2,4,6-trimethylbenzoic acid, or otho-dichlorobenzene. The conversion is reported at 47% with a selectivity of >98% to methyl-3-pentenoate and 1.8% to methyl-2-pentenoate. In US 5495041 and US 5693851, a similar reaction takes place with a mixture of butadiene, methanol and a protonic acid, such as 2,4,6-trimethylbenzoic acid or 3-pentenoic acid, in diphenyl ether. The conversion of butadiene is 75-95% after 2-5 hours of reaction with a selectivity of 79-96% to methyl pentenoates. The molar ratio of the protonic acid to Pd catalyst is 10:1. About 46-70% of the pentenoic acid is converted to methyl ester during the reaction. To maintain a catalytically active level of pentenoic acid in the reactor mixture, a part of the methyl pentenoate in the reactor effluent is hydrolyzed to the acid, which is recycled to the reactor.

The methyl pentenoates are hydroformylated to methyl-5-formylvalerate (M5FV) as shown in reaction 4.3 in the presence of a rhodium carbonyl catalyst and a phosphine ligand, such as tris(m-sulfonato-phenyl)phosphine (US 5719312, US 5527950). The reaction takes place at 90-110°C and 1.0 MPa. The conversion of methyl pentenoates is about 50% after more 20 hours of reaction at 90°C or 80% at 110°C. The selectivity to M5FV is < 80%.

M5FV, its methyl ester or a mixture thereof is subjected to reductive ammoniation to form a mixture of CAPM and its precursors, such as methyl-6-aminocaproate (M6AMC), 6-aminocaproic acid (6AMCA), and 6-amino-caproamide (6ACAM). The composition of the reaction mixture varies, depending on the reaction conditions and the type of catalyst employed for the reaction. In a process cited in US 5717089 and US 5700934, M5FV is subjected first ammoniation without a hydrogenation catalyst followed by reductive ammoniation in the presence of Ru catalyst supported on alumina or Raney nickel catalyst. The conversion of M5FV is complete with > 99% selectivity. The same catalysts are used in one-step reductive ammoniation with similar results (US 5780623, US 5973143). The reaction effluent is distilled to remove methanol and ammonia before it is subjected to cyclization. However, these catalysts are not chemically and mechanically strong, and the catalyst particles broken down along with decrease in catalyst activity after a short running time (US 5877314).

In US 5877314, the reductive ammoniation is performed by contacting M5FV in aqueous solution with hydrogen and excess ammonia in a Hastelloy-C autoclave with suspended Ru catalyst supported on titanium oxide. The reaction takes place at 120°C and 4 MPa. After 1 hour of reaction, the M5FV is completely converted with 97% selectivity to CAPM and its precursors. The use of TiO₂ is preferred because of its high chemical resistance and mechanical stability. A catalyst with a higher BET surface area of 48 m²/g provides a 3.5 time higher catalyst activity than the one with 3.4 m²/g BET surface area.

Cyclization of 6AMCA, 6ACAM and M6AMC

The reaction effluent from the above reductive ammoniation comprises about 75 wt% water with remainder of organic compounds, which contains a mixture of CAPM and its precursors. The aqueous mixture is concentrated to remove most of the water through a film evaporator from 75 wt% to less than 25 wt%. The resulting solution is then cyclized to produce CAPM. In US 6194572, cyclization is carried out at 300°C and 1.2 MPa by contacting with a superheated steam. After 5 hours, the organic compounds are completely converted with > 99% selectivity to CAPM. The cyclization effluent is distilled in a series of two columns under vacuum to remove water and ammonia through the first column. CAPM is obtained as a distillate from the second column, and the residue from the second column is recycled to the cyclization reactor (US 6011153).

In a process described in US 5502185, 6AMCA is cyclized in a fixed-bed reactor packed with TiO₂ extrudate. The reaction takes place at 220°C and 10 MPa with a solution of 6AMAC in a

mixed solvent of ethanol and water with a weight ratio of ethanol to water greater than 50:40. A conversion of 97% is reported after 15-min residence time with selectivity to CAPM at 93%. A longer residence time provides a higher conversion but decreasing selectivity. A higher ethanol content also provides better conversion and selectivity.

Cyclization 6-aminocaproic acid (6AMCA) in the presence of methanol, which is formed during the hydrolysis of methyl 5-formylvalerate, produces an undesirable amount of N-methyl caprolactam (US 5973143, US 5780623). This by-product is difficult to be separated from CAPM, and will cause undesirable quality in nylon 6 fibers. Therefore, it is preferable to subject the reaction mixture of AMCA production to steam stripping to remove methanol before it undergoes cyclization to produce CAPM.

In US 6194572, an aqueous mixture of 6AMCA, its methyl or ethyl ester, and/or 6ACAM is subjected to cyclization by contacting with a superheated steam with a weight ratio of steam to the aqueous mixture between 1:1 and 20:1. The reaction product is withdrawn as a vapor containing CAPM, steam and some ammonia when 6ACAM is present in the aqueous mixture. The mixture can be obtained from a combined hydrolysis and reductive ammoniation (US 5973143, US 5780623), or from 6AMCN as mentioned above.

Purification of Caprolactam

From the technology review presented above, crude CAPM can be derived from the following four different processes:

- Liquid-phase Beckmann rearrangement
- Gas-phase Beckmann rearrangement
- Cyclization of an aqueous mixture from reductive ammoniation of M5FV and its methyl ester
- Cyclization of 6AMCN

The crude CAPM from the liquid-phase Beckmann rearrangement is typically neutralized with aqueous ammonia. The resulting mixture is decanted to obtain aqueous crude CAPM, which goes through extraction with benzene followed by water wash. The extraction operation can be conducted more than one time (US 5539106). The washed crude CAPM is then subjected to ion exchange followed by hydrogen treatment at 80°C in the presence of water and a Pd catalyst supported on activated carbon. The treated aqueous CAPM is finally concentrated by evaporation followed by distillation.

As mentioned earlier, ethanol or methanol is used along with water as the solvent for cyclohexanone oxime in the gas-phase Beckmann rearrangement. The reaction effluent is cooled and condensed to obtain crude CAPM Crude, which is distilled to remove alcohol, light ends and heavy ends. The resulting CAPM having a purity of 98.97 wt% with impurities of 584 ppm cyclohexanone oxime, 604 ppm of 3-N-methyl-4,5,6,7-tetrahydrobenzimidazole, and 355 ppm of 1,2,3,4,6,7,8,9-octahydrophenazine is further purified by crystallization followed by hydrogenation treatment (US 6252068). CAPM from Beckmann rearrangement with oleum in liquid-phase reaction contains by-products, which are different from those from gas-phase Beckmann rearrangement with a solid catalyst. In the former case, the hydrogen treatment is carried out at 50-80°C for producing high quality CAPM, while in the latter case the treatment is carried out at 80-95°C (US 6252068 B1, US 5502184). The treated CAPM is further distilled to get a purity of 99.998 wt%.

Purification of the crude CAPM from cyclization of 6AMCN is relatively simpler than the conventional crude CAPM from the liquid-phase Beckmann rearrangement because it does not

require decantation to remove aqueous ammonium sulfate and extraction operation afterwards. The crude CAPM is first distilled to remove ammonia along with some ethanol and water. It is further distilled to remove the remaining mixture ethanol and water, light ends and heavy ends. The resulting CAPM is hydrogenated at 90°C followed by ion exchange with acidic ion exchanger at 50°C. The resulting CAPM is further distilled to remove water, and remaining light ends and heavy ends to obtain CAPM with high purity (US 5496941). The light ends are essentially ethyl 6-amoniocaproate (E6AMC) and unconverted 6AMCN, while the heavy ends are 6ACAM, 6AMCA and oligomers (US 5874575, US 5693793). The light ends can be recycled to the cyclization reactor or incinerated. The heavy ends can be subjected to depolymerization treatment in the presence of phosphoric acid (US 5874575), or in a fixed reactor packed with TiO₂ extrudate (US 5495014) to recover CAPM. In US 6194572 and US 6100396, crude CAPM leaves the cyclization reactor as a vapor. It is condensed and distilled to remove ammonia and some water. The resulting CAPM solution can be purified by similar procedures described above. Alternatively, it is either extracted with a mixture of 30 wt% bis(2-ethylhexyl)hydrogen phosphate and 70 wt% cyclohexane or treated with macroporous sulphonic resin with a solution to resin ratio of 0.3:1 in equivalent to remove most of by-products (US 6100396). The resulting treated CAPM is further purified by distillation.

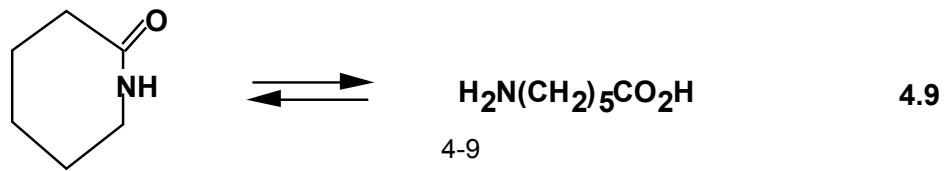
Technology for Nylon 6

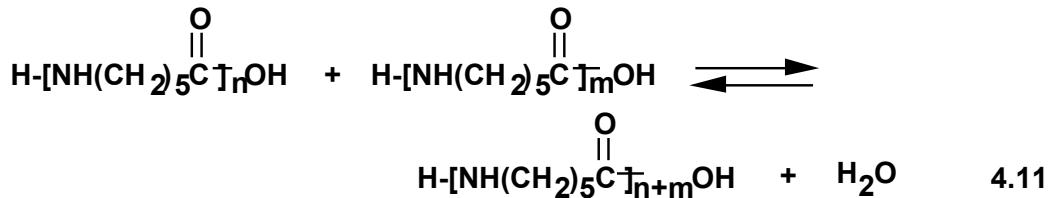
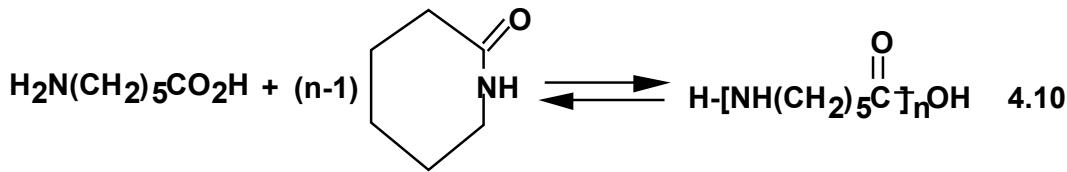
Commercially, two polymerization processes are used to manufacture nylon 6, i.e. hydrolytic polymerization and anionic polymerization. The former is mostly employed for making nylon 6 for fiber and film production, while the latter is used mostly for making nylon 6 for extrusion and castings. A list of patents for the hydrolytic polymerization is given in Table 4.2 and those for the anionic polymerization are given in Table 4.3.

Hydrolytic Polymerization

Hydrolytic polymerization is the most important method for the production of nylon 6 at present. A typical commercial process involves essentially three stages. Initially, CAPM is hydrolyzed with water in the presence of phosphoric acid (JK 11343338) to open the ring, resulting in formation of aminocaproic acid, which then reacts with CAPM through addition polymerization (polyaddition) to generate prepolymers with amino and carboxyl end groups. The polymer chains of the prepolymers are then extended by condensation polymerization (polycondensation) to produce nylon 6 with desirable MW as shown in reactions 4.9 through 4.11. In reality, both polyaddition and polycondensation occur in the process after initial ring opening reaction, with the former prevalent in the second stage, and the latter prevalent in the third stage. While the ring opening reaction is endothermic, both the polyaddition and polycondensation are exothermic.

It is known that the polycondensation reaches a chemical equilibrium, which is temperature-dependent. In general, the polymer yield decreases with the increase in reaction temperature because the reaction equilibrium shifts towards the formation of cyclic and linear oligomers (240020). Raising the temperature, however, will increase the polymerization rate, and reduce the time required to reach equilibrium. The optimum reaction temperature ranges from 260 to 280°C. In a common plant, the reaction temperature of 280°C provides nylon 6 resin with about 13 wt% water soluble fraction, including CAPM, dimers and oligomers. Either water extraction or vacuum stripping with inert gas if necessary removes this low MW fraction from the resin.





In US 6069228, an aqueous 80 wt% CAPM solution is fed into a vertical coiled tubular (or pipeline) reactor at < 270°C and 2.86 MPa, which is below the solution vapor pressure so that a mixture of gas and liquid phases exists in the reaction mixture. The conversion of CAPM is 85% over a residence time for the liquid prepolymer of 35-40 min. The reactor effluent passes to a separator via a horizontal coil flasher. The molten prepolymer is crystallized on a temperature controlled steel belt. The crystallized prepolymer is subjected to solid-phase polymerization in a vertical tubular reactor with a conical bottom section. The polymer flow downward countercurrently with heated nitrogen gas at 160°C.

The nylon 6 granules from conventional polymerization generally contains about 8-15 wt% unreacted CAPM and oligomers. They are continuously extracted in a vertical extraction column having two operation zones to remove the extractables from nylon 6. An aqueous CAPM solution having 20-30 wt% CAPM (WO 9926998) or 75-95 wt% (WO 9926996) is used as an extraction agent for the top zone at 115-130°C, while water is fed to the lower end of the bottom zone at 20-30°C. The top operation zone of the extraction column has larger cross section area than the bottom operation zone with a diameter ratio of the two at > 1.3:1. The bottom zone, however, has longer length than the top zone at a ratio of >5:1 (WO 9926998). Both zones are equipped with heating jackets. In WO 9926996, an unheated slender tube is used for the lower zone.

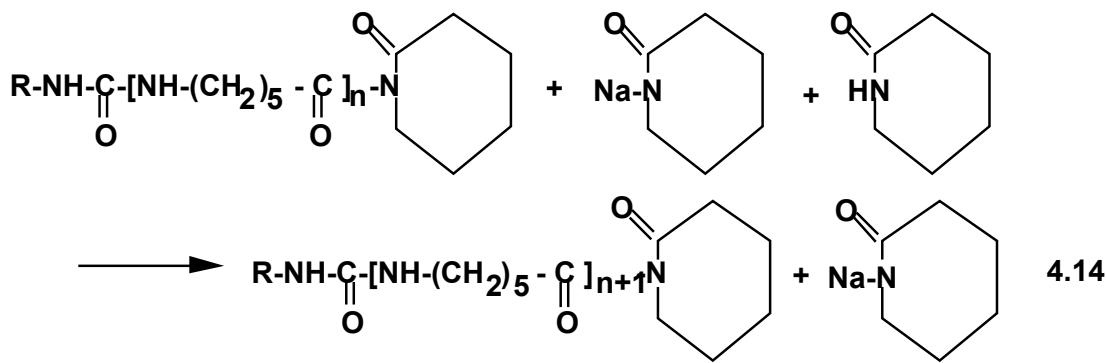
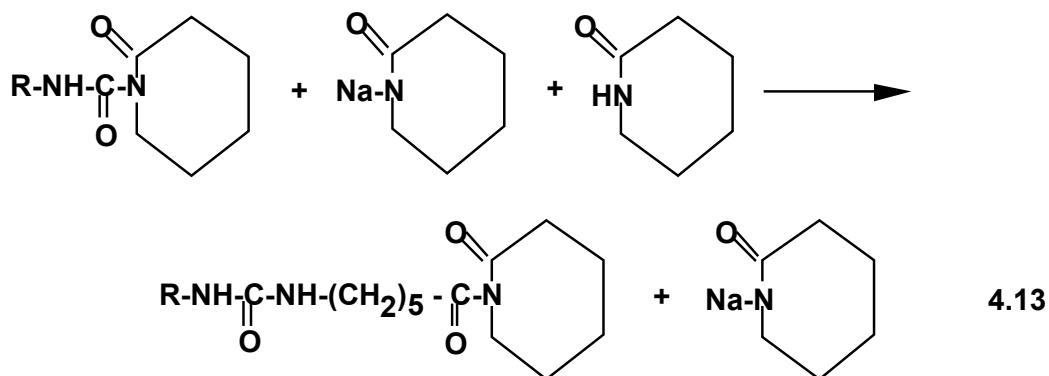
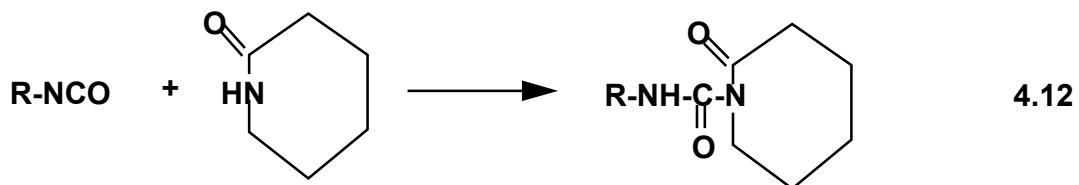
The aqueous extract is concentrated by distillation and/or evaporation to >90 wt% before it is recycled to polymerization (US 4816557, EP 167975 A2). In US 6093788, The extract water is first concentrated from about 8 wt% to 70 wt% by means of multi-stage distillation. The concentrated extract water is further distilled or evaporated to recover a CAPM/water mixture, and to yield an extract containing 33-67 wt% CAPM and 67-33 wt% oligomers (including dimers). The latter is depolymerized in the presence of a catalyst and superheated steam to generate a vaporous mixture of 16-33 wt% CAPM and 84-67 wt% water (US 5973105, US 5962538), which is condensed and combined with the CAPM/water mixture from earlier evaporation. The resulting CAPM/water mixture is distilled to yield CAPM with a water content of less than 4 wt% and a dimer content of not greater than 0.05 wt%.

Anionic Polymerization

Anionic polymerization of lactam is carried out in the presence of a catalyst and an initiator. The lactam is generally CAPM with a higher lactam, such as laurolactam, can be incorporated as copolymers with modified characteristics. Most of anionic polymerization of CAPM reported in the

literature employs sodium caprolactamate as the catalyst, which is dissociates into a lactam anion and isocyanate/CAPM adduct as the initiator. Other initiators, N-acyllactams are prepared from the reaction of a lactam with either an anhydride or an acid chloride. Various catalysts reported include Grignard reagents and lactam salts prepared from lactam and compounds, such as alkali aluminum hydride and quaternary ammonium halide.

The polymerization begins with the formation of a chain extended lactam anion between the initiator and the lactam anion. The chain extended lactam anion then reacts with CAPM to regenerate the lactam salt and a chain extended compound with an N-acyllactam end group. The Chain growth reaction proceeds with formation of a new chain extended lactam anion and etc. as shown in reactions 4.12 through 4.14. A few patents are listed in Table 4.3.



Traditionally, the anionic polymerization is carried out by separately prepared CAPM melts of equal volume, each of which contains the catalyst and activator, respectively. They are mixed and processed under an inert gas. The disadvantage of using these solid catalysts is the

formation of an inhomogeneous polymer unless rapid dissolving and even distribution of these components in the CAPM melts are assured. A catalyst/activator system comprising 45-70 wt% N-substituted carbonamide, such as N-alkyl-2-pyrrolidone, 5-30 wt% alkali and/or alkaline earth caprolactamate, 10-40 wt% activator, such as lactam-blocked diisocyanate, and 0.5-30 wt% N-substituted urea is cited to remedy this difficulty (US 5760164, US5747634, AU 722606). In this system, both N-alkyl-2-pyrrolidone, such as N-methyl-2-pyrrolidone, and N-substituted urea, such as tetrabutyl urea, tetraethyl urea or tetramethyl urea, are solvents, in which sodium caprolactamate and lactam-blocked diisocyanate are dissolved. The liquid catalyst/activator system is prepared by adding a lactam-blocked methylene diisocyanate into the solvent. The resulting mixture is heated to 30-70°C to dissolve the activator. After clear solution is formed, the caprolactamate is added and mixed with the temperature of the mixture not exceeding 70°C. The polymerization is carried out by introducing the liquid system to a CAPM melt while stirring under nitrogen over a period of one minute or less. The resulting mixture is then polymerized at 140°C for about one hour.

REVIEW OF TECHNOLOGY FOR NYLON 66 AND ITS PRECURSORS

Table 4.4 presents an annotated list of patents for technology for preparation of ADA, while Tables 4.5 summarize the patents for HMDA. Patents pertaining to the technology for the production of nylon 66 are listed in Table 4.6

Technology for Adipic Acid

In PEP report 3B (November 1996), we reviewed various routes to produce ADA from benzene, cyclohexane and butadiene. In the following, we review current development of these technologies.

Adipic acid from benzene

Benzene can be partially hydrogenated to cyclohexene, which is subjected to hydration followed by oxidation to produce ADA. In 1999, Asahi Chemical commercialized this process in Japan, which is only commercial plant using this technology at present. Alternatively, the cyclohexene can react with ADA to form cyclohexyl adipate, which is then oxidized to ADA.

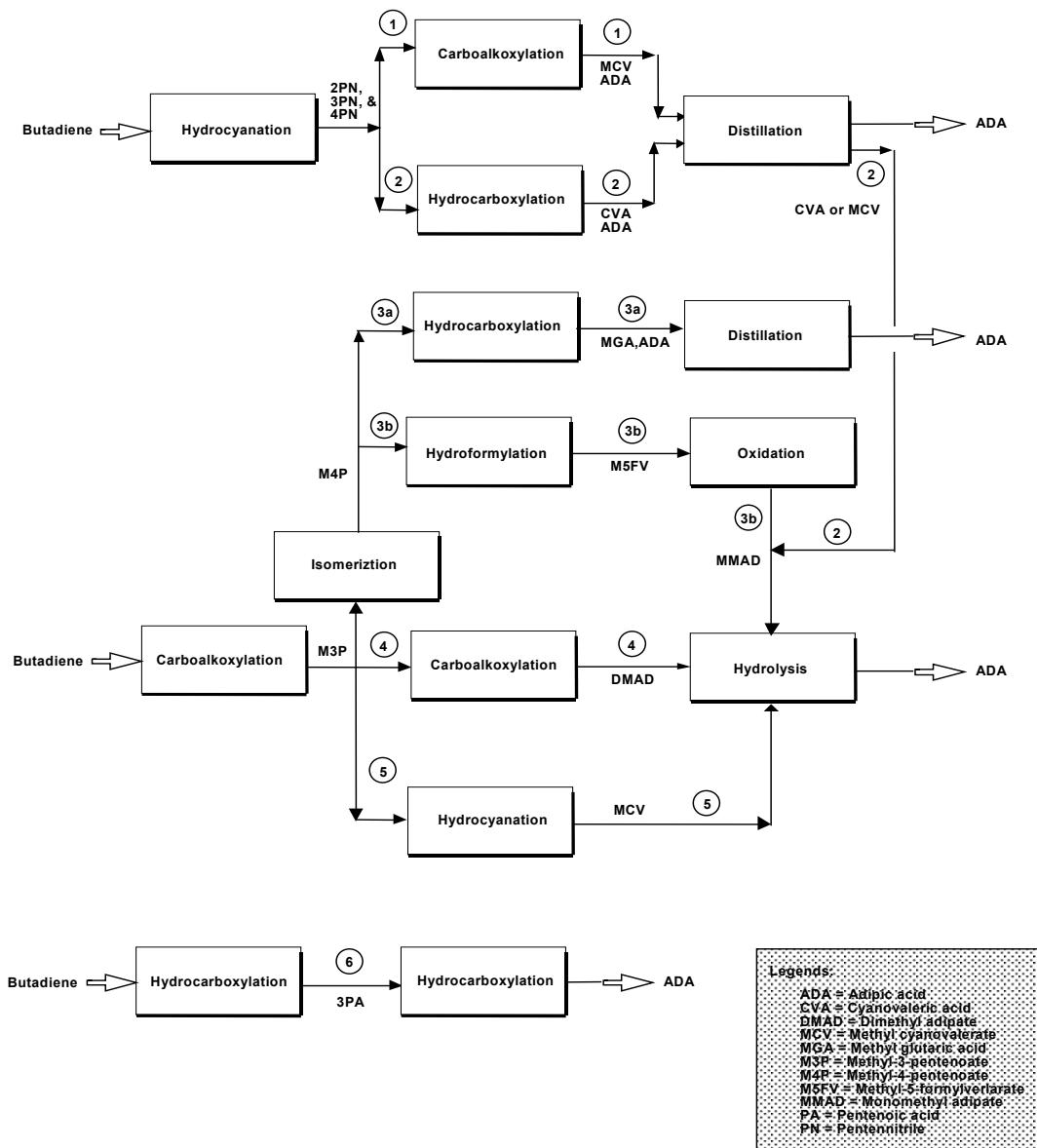
In US 5973218, the activity of a Ru Catalyst can be maintained over a period of 1600 hours when ZnSO₄ is used as a promoter and kept at its concentration initially at 0.5 and increased to 0.8 mol/l. The reaction takes place 130°C and 5 MPa with the conversion of benzene reaching up to 70% and the selectivity to 82-85%. The Ru catalyst can also be either modified with nickel (US 5589600) or supported on ZrO₂ modified silica (US 5639927, US 5569803). In the former case, the catalyst is promoted with ZnSO₄ and ZrO₂ to improve the selectivity. In the latter case, the catalyst is pretreated with ZnSO₄ or Li₂SO₄ at 150-200°C for 5 hours followed by hydrogen treatment. The treated catalyst is washed with water and dried. The dried catalyst is further treated with hydrogen at 200°C for 2 hours before it is used for the reaction. The conversion of benzene is improved from less than 30% to 63% while the selectivity is kept at about 78%.

The reaction mixture of partial hydrogenation of benzene contains cyclohexene, cyclohexane, and unreacted benzene. Cyclohexene is recovered from this mixture by extractive distillation with 1,3-dimethyl-2-imidazolidinone serving as an extraction solvent. A series of four distillation columns is cited for the recovery (US 5865958).

Adipic acid from butadiene

There are several routes to prepare ADA from butadiene. PEP Report 3B presented a detailed review of these technologies. Figure 4.1 shows major routes for manufacturing ADA from butadiene reviewed in that report.

Figure 4.1
**BLOCK DIAGRAM OF MAJOR ROUTES FOR MANUFACTURING
 ADIPIC ACID FROM BUTADIENE**



- Route 1 -- Butadiene can be hydrocyanated to a mixture of 3-pentene-nitrile (3PN) and 4-pentenenitrile (4PN). The pentenenitriles are subject to hydrocarboxylation to form ADA with methyl cyanovalerate (MCV) as a major by-product. MCV is separated from ADA by distillation followed by hydrolysis to generate more ADA.
- Route 2 -- Butadiene can be hydrocyanated to a mixture of 3-pentenenitrile (3PN) and 4-pentenenitrile (4PN). The pentenenitriles are subject to carboalkoxylation to form ADA with cyanovaleic acid (CVA) as a major by-product. CVA is separated from ADA by distillation followed by hydrolysis to generate more ADA.
- Route 3 -- Butadiene can be carboalkoxylated to form methyl-3-pentenoate (M3P). M3P can be isomerized to methyl-4-pentenoate (M4P), which is then converted to ADA by the following alternatives.
 - Route 3a -- M3P can be first isomerized to methyl-4-pentenoate (M4P), which is then hydrocarboxylated to ADA with methyl glutaric acid (MGA) as a major by-product. ADA is recovered by distillation or crystallization.
 - Route 3b -- M3P can be first isomerized to methyl-4-pentenoate (M4P), which is then hydroformylated to methyl-5-formylvalerate (M5FV). The latter is subject to oxidation to produce monomethyl adipate (MMAD), which is hydrolyzed to ADA.
- Route 4 -- Butadiene can also be carboalkoxylated to form methyl-3-pentenoate (M3P), which is then further carboalkoxylated to produce dimethyl adipate followed by hydrolysis to ADA.
- Route 5 -- Butadiene can be carboalkoxylated to form methyl-3-pentenoate (M3P), which is then reacted with HCN to produce MCV followed by hydrolysis to ADA.
- Route 6 -- Butadiene can be hydrocarboxylated to 3-pentenoic acid (3PA), which is then further hydrocarboxylated to ADA.

Among these routes, the first three routes are more complicated, and/or overall yields of adipic acid are not desirable. The second three routes are more straightforward. Among them, Route 4 provides relatively higher overall yield than Routes 5 and 6. Route 4 was presented in PEP Report 54B and updated in PEP Report 3B with modification based on the information reviewed in the latter report. So far, this process has not been commercialized.

Table 4.4 presents a list of patents pertaining to hydrocarboxylation of butadiene to form pentenoic acids, which in turn are further hydrocarboxylated to ADA. The first stage of hydrocarboxylation is carried out in an organic solvent, such as acetic acid or ADA, in the present of a Rh, Ni or Ir catalyst with HI as a promoter (US 6133477, US 5962732, US 5763655, US5166421, US5145995). Halocarbon solvents, such as methylene chloride appears to hydrolyze, forming products that react with butadiene to lower the yield to ADA (US 5145995). The molar ratio of promoter to the catalyst is critical to obtaining the high rates of reaction and the yield of ADA. Reportedly the preferable ratio ranges from 2:1 to 6:1. The reaction can also be carried out in the presence of a crotyl/Pd chloride complex with excess crotyl chloride as co-catalyst (US 5625096). The reaction takes place at 140-200°C and 3.5-5.0 MPa when the Rh is employed. A relatively high pressure is cited when the other catalysts are used. The conversion of butadiene is reported at greater than 90% when the Rh and Ni catalysts are used with selectivity to pentenoic acids mostly at 87-95%. The Ir catalyst provides relatively low yield of pentenoic acids.

In the second stage of hydrocarboxylation, pentenoic acids, mostly 3-pentenoic acid (3-PA), reacts with CO and water in the presence of a Rh or Ir catalyst also promoted with HI. It is reported that nonpolar solvents, such as cyclohexane and toluene, are undesirable because of

their propensity to promote the formation of branched dicarboxylic acids and saturated monocarboxylic acids (US 5198577). Carboxylic acids, such as acetic acid and ADA are cited in the patents to serve as the solvent for the reaction. The former, however, provides low linearity* of the final products (US 5198577). The use of ADA as solvent provides improved conversion and selectivity (US 5227522). When the reaction is carried out in absence of solvent, it results in poor conversion and selectivity (US 5312979). The reaction takes place at 170-190°C and 1-5 MPa. A conversion greater than 90% is reported in several cases (US 5420346, US 5266505, US 5227523, US 5227522, US 5198577), however, with low selectivities ranging from 50 to 75%.

Adipic acid from cyclohexane

Conventionally, ADA prepared from cyclohexane is subjected to two steps of oxidation. In the process, cyclohexane is first catalytically oxidized to a mixture of cyclohexanone and cyclohexanol (KA oil), which is further oxidized to ADA by using nitric acid as an oxidant. The latter generates nitrogen oxides, which requires necessary treatment to avoid any environmental contamination. The first stage of oxidation takes place generally at 130-160°C with the oxygen level in the gas phase of the oxidation reactor kept below a flammability limit, which is slightly above 1%. The conversion of cyclohexane is kept low at 3-5 % in order to achieve desirable selectivity to KA oil. The reaction also produces by-products, such as cyclohexyl hydroperoxide (CHHP), acetals, ketals and cyclohexyl esters of monocarboxylic and dicarboxylic acids. Several approaches have been cited to decompose CHHP into KA oil. The decomposition reaction takes place at 62-90°C in the presence of a Co catalyst and an aqueous solution of NaOH Na₂CO₃ and NaHCO₃ (US 5959153, US 5905173, US 5892122, US 5859301). The Co catalyst can be Co-acetate and/or Co-sulfate, and it can be a heterogeneous catalyst supported on TiO₂ or a homogenous catalyst. The reaction can also be carried out at a relatively higher temperature of 125-150°C in absence of the aqueous caustic solution in the presence of a heterogeneous catalyst selected from Au, Ag or Cu (US 6284927) or from Ti Zr, or Nb (US 6191311) supported on silica.

In US 6008415, an oxygen-enriched air or pure oxygen is used for the oxidation reaction so that the reaction can be operated at a relatively lower temperature than that in the conventional reaction (149 versus 160°C) using air as the oxidant. Reportedly, the selectivity to KA oil is improved from 62 to 74% and residence time is reduced from 36 to 8 minutes. The reactor is equipped with a hollow shaft chamber, and helical impeller means, which is positioned inside the chamber and provide a downward flow of the reaction mixture through the chamber and upward flow through the annular area between the reactor wall and the outside wall of the hollow chamber. A baffle with a number of opening is positioned a short distance below the gas-liquid interface to keep most oxygen bubbles within the main reaction body with the help of attached guide baffle means. To keep the oxygen concentration in the gas phase above the gas-liquid interface below the flammability limit, inert gas let means are provided below and above the perforated baffle. The oxygen-enriched air is fed to a lower position inside the hollow chamber.

The direct oxidation of cyclohexane has been worked at by the industry for a long time, on account of the obvious advantages of converting cyclohexane into ADA in a single step without using the nitric acid. However, the conversion and selectivities reported in the past have not been industrially economical. Recently, a direct oxidation process is cited in US 5900506, in which the reaction takes place at 105°C and 2.0 MPa in the presence of Co-acetate·4H₂O. Both conversion and selectivity still remain low.

* Linearity is measured by the degree of branched dicarboxylic acids formed during the reaction.

Purification of Adipic acid

As reviewed previously, ADA can be prepared from butadiene by two-step hydroxycarbonylation, from cyclohexane by oxidation or from benzene by partial hydrogenation and oxidation. The impurities contained in ADA thus prepared are different, particularly between the butadiene-based process and the other two processes. The impurities from the butadiene-based process include 2-methylglutaric acid, 2-ethylsuccinic acid, dimethylsuccinic acid, and other compounds originating from the first-step hydroxycarbonylation, such as γ -valerolactone methyl butenoic acid, pentenoic acids and the Ir and/or Rh catalyst. Those from the other two processes are monobasic acids, dibasic acids, various esters thereof and the Co, Cu and/or other catalysts. The amounts of these impurities depend on the conditions under which the reaction is carried out.

There are various approaches to recover and purify ADA from the reaction products. In US 5587511 and US 52102297, The crude ADA from oxidation of KA oil is subjected to crystallization to remove ADA. The mother liquor is distilled or evaporated to remove nitric acid along with water. The concentrate is heated to 150-160°C and 15-95 kPa to decompose and remove the nitrogen compounds before it is dissolved in water (US 5210297). The resulting aqueous solution is treated with cation exchange resin to separate the catalyst ions before it is subjected to evaporation to remove the water, and distillation to obtain a mixture of dicarboxylic acids. The latter mixture is suitable to prepare polyesterpolyols. Alternatively, the concentrate is mixed with water or dilute nitric acid; the mixture is heated at 70°C for about 10 minutes before it is cooled to recover ADA crystals thereof (US 5587511). In DE 440916 and 4440733, the crude ADA is extracted with a solvent, such as MIBK or cyclohexane to remove Co catalyst, and washed with water before it is crystallized to recover ADA.

In WO 00/15597 and WO 99/44980, the reaction product from the direct oxidation of cyclohexane in acetic acid is decanted to separate unreacted cyclohexane in the upper layer. The lower layer is distilled to remove the solvent and residual cyclohexane before the distillation residue is washed with water or other solvents and cooled to crystallize ADA. In this case, the crystallization is carried out in the presence of a strong acid such as HI, HBr, HCl or sulfuric acid and/or CO to reduce the catalyst content in the purified ADA (US 6222069, WO 97/465510, WO 97/465509).

In the reaction products from the two-step hydrocarboxylation of butadiene, the crude ADA contains 2-methylglutaric acid, 2-ethylsuccinic acid, dimethylsuccinic acid, and other compounds originating from the first-step hydroxycarbonylation as mentioned earlier. It is very difficult to separate these dicarboxylic acids (or diacids) from ADA because of the very close physical properties among these compounds. In US 5587056, these branched diacids are dehydrated to form anhydride in the presence of to permit a more ready separation thereof from the ADA in the mixture because of the much lower boiling points of these anhydrides relative to their respective diacids.

Treatment of Nitrogen oxides

In the oxidation of KA oil with nitric acid, the reaction produces nitrogen oxides as a waste gas, which typically comprises 20 vol% NO₂, 23 vol% N₂O, 10 vol% O₂, 2 vol% carbon oxides, and the remainder of nitrogen and some inert gas, such as Ar (US 6056928). The gas mixture is initially subjected to absorption at 30-40°C with water or dilute nitric acid in the presence of free oxygen to remove nitrogen oxides other than dinitrogen oxide. The gas stream from the absorption is heated to 450-500°C before it is catalytic reduced with ammonia to nitrogen and water. Other catalysts can be zeolites, which have been exchanged metals, such as Fe, Co, Cu, Rh, Pd, or Ir (US 6056928, US 5582810).

Technology for Hexamethylenediamine

Commercially, hexamethylene diamine (HMDA) is mostly produced from butadiene by liquid-phase catalytic hydrocyanation to form pentenenitriles, which is further hydrocyanated to produce adiponitrile (ADN). The latter is hydrogenated to HMDA. Alternatively, ADN is prepared from acrylonitrile (ACN) by electrohydromerization. Currently, there may be a few plants in Eastern Europe using ADA-based process for ADN by ammoniation of ADA followed by dehydration.

Table 4.5 summarizes a list of patents pertaining to technologies for HMDA. The hydrocyanation of butadiene proceeds in the presence of transition metal complexes with mono- or bidentate phosphite ligand without the use of a Lewis acid promoter. But a Lewis acid promoter is required when 3-pentenenitrile (3-PN) is hydrocyanated.

As presented in Table 4.1, HMDA is also a co-product in the partial hydrogenation adiponitrile to prepare 6AMCN, which is cyclized to form CAPM.

Hydrocyanation of Butadiene

A nickel-ligand complex is used as the catalyst for the hydrocyanation of butadiene. The complex can be prepared by reacting bis(1,5-cyclooctadiene)nickel(0) with a bidentate metallocene-phosphorus(III) ligand (US 6169198), various bidentate phosphite ligands (US 5693843, US 5449807, WO 99/64155) or multidentate phosphite ligands (US 6171997, US 6120700, US 5821378, US 5696280). Some of these ligands are supported on an insoluble polymer through reaction of various phosphorochloridites with a supported diol resin (US 6121184).

The reaction of hydrocyanation of butadiene in liquid phase takes place at 80-90°C under autogenous pressure or at 145-150°C in gas phase. The conversion of butadiene reportedly high at > 90% over a period of >3 hours with a selectivity to 3PN and 2-methyl-3-butenenitrile (2M3BN) ranging from > 95%. However, in most the cases, the molar ratio of 3PN to 2M3BN in the reaction product is relatively low ranging from 0.22:1 to 1.72:1, except when the metallocene-phosphorus(III) ligand is used, a molar ratio of 24:1-30:1 is reported. Therefore, there is a need of a second reaction to isomerize 2M3BN to 3PN.

Isomerization of 2M3BN takes place at 110-125°C in liquid phase in the presence of same catalyst system used the hydrocyanation reaction with a conversion > 94% and a selectivity 95-99% (US 6171997, US 6120700, US 5821378, US 5696280). It also can be carried out in gas phase at 145-150°C (US 5440067). However, the selectivity to 3PN is low at about 78%. Alternatively, the phosphorous ligand is replaced with trisulfonated triphenylphosphine, and the reaction takes place at 90°C (US 5486643). The conversion is 87-95% with a selectivity of 91-94%.

Hydrocyanation of Pentenenitrile

Like the nickel-ligand complexes cited for the hydrocyanation of butadiene, the nickel-ligand complexes for the hydrocyanation of 3PN also comprise bidentate phosphite ligands (US 5723641, US 5688986, WO 99/52632), and multidentate phosphite ligands (US 6171996, US 5959135, US 6127567, US 6020516, US 5981772, US 5847191, US 5663369, US 5512696). All these catalyst systems cited use ZnCl₂ as promoter for the reaction, which takes place at 50-70°C. The conversion for the hydrocyanation reaction varies from 33% to 95%, depending on the stereospecific character of groups linked to the phosphorus atom in those ligands. The selectivity to ADN is less affected, varying from 70% to 97%.

Water soluble monodentate phosphine ligands, such as sodium salts of 1,2-bis[di(sulfonatophenyl)-phosphinomethyl]cyclobutane, tris(sulfonatophenyl)-phosphine, tris(para-phosphophenyl)-phosphine, bis(meta-sulfonato-phenyl)(para-carboxyphenyl)phosphine, and bis(metasulfonatophenyl)(2-sulfonatoethyl)phosphine, are cited in US 5856555 and US 5488129 for hydrocyanation of 3PN in the presence of Ni(0) catalyst. A Lewis acid, such as ZnCl₂, FeCl₂, SnCl₂, or mixture thereof, is used as a promoter. The reaction takes place at 60-65°C with 69-81% yield to ADN.

In a conventional hydrocyanation process, 3-PN is converted to ADN in the presence of Ni(0) catalyst with triarylborane as a promoter. During the reaction, some Ni(0) catalyst is oxidized to Ni(CN)₂, which forms insoluble complex with the promoter. This complex causes encrustation on equipment surfaces, resulting in inefficient heat transfer through the equipment wall. It may also cause difficulties in catalyst recovery if the insoluble complex suspended in the reaction mixture. In US 4990645, an improvement of this process is cited. The improved process is to control HCN concentration in the product stream at < 2500 ppm, and to recycle part of solid catalyst degradation precipitate to the hydrocyanation reactor in order to minimize the fouling of process equipment caused by solid catalyst degradation precipitate. In the process, the reaction effluent is subjected to flashing to remove unconverted pentenenitriles. The crude ADN is then decanted with part of the lower phase, which contains solid catalyst degradation precipitate, is recycled to the hydrocyanation reactor. The remainder is discarded after washing with PN to recover the retained catalyst. The upper phase from the decanter is extracted with an organic solvent to remove the catalyst and ligand from ADN product. The catalyst in the extract is then separated from the solvent and recycled to the reactor.

Hydrogenation of Adiponitrile

ADN is conventionally hydrogenated at about 140°C and 30 MPa in the presence of reduced Co or iron oxide with complete conversion and a high selectivity to HMDA. The reaction, however, requires a large amount of ammonia in the reaction mixture; therefore, the excess ammonia has to be recovered and recycled. In US 5900511, Raney Co doped with metals, such as Cr and Ni is used for the hydrogenation at 75°C and 3.6 MPa. An aqueous ammonium hydroxide is intermittently added to rejuvenate the catalyst. ADN is completely converted during the reaction with selectivity to HMDA at 97-99%. Raney nickel doped with Ti or Cr is used for the hydrogenation of ADN in a mixed solvent of ethanol and water (US 5840989, US 5801286, US 5777166). The reaction is carried out at 80°C and 2.5 MPa in an autoclave in the presence of a small amount of caustic soda. The selectivity to HMDA is reported at 95-97% at 100% conversion.

Ruthenium complexes, such as RuH₂(N₂)₂(PCy₃)₂, RuH₂(H₂)₂(PCy₃)₂, RuH₂(N₂)₂ (P-iPr₃)₂, and RuH₂ (H₂)₂(P-iPr₃)₂, are cited in US 5726334, US 5599962 and US 5559262, where Cy is a cyclohexyl group. These complexes are prepared from Ru(COD)Cl₂ (COD is 1,5-cyclooctadiene) and phosphine, such as PCy₃ or P-iPr₃, in the presence of NaOH, benzyltriethylammonium chloride (as phase-transfer catalyst) and a solvent selected from benzene and toluene. The reaction takes place at 80-100°C and 7 MPa, and requires a reaction time of greater than 8 hours to achieve >99% conversion and > 94% selectivity to HMDA.

As reviewed earlier, the reaction mixture from partial hydrogenation of ADN comprises HMDA, 6AMCN, unreacted ADN, ammonia, water and small amounts of other by-products, such as hexamethyleneimine, 2-aminomethylcyclopentylamine, and 1,2-diaminocyclohexane. In US 6139693, HMDA is reportedly to be recover from the mixture by distillation in a series of 3 or more columns. No specific description of distillation is given.

Technology for Nylon 66

Nylon 66 is traditionally prepared by polycondensation of adipic acid and hexamethylenediamine into an aqueous AH (nylon 66) salt solution, generally at about 50 wt%. The solution is then used as an initial reaction medium for the solution/melt polymerization to produce nylon 66. Such an operation requires high-energy consumption and is time consuming. Recently, various approaches have been considered to avoid this expensive and complex process.

In US 5801278, AH salt is produced in the presence of much small amount of water at 2-5 wt% based on the weight of the reaction mixture. The salt produced is less dangerous than the 90 wt% HMDA solution, which is a typical shipping form for the diamine. Theoretically, an equal molar ratio of ADA to HMDA is used to produce AH salt. In practice, the ratio can be adjusted as desired; for example, additional HMDA is incorporated into a salt for the manufacture of nylon 66 fiber, which requires increased dyeability for anionic dyes. In US 6011134, HMDA reacts with monomethyl adipate in an equimolar ratio in the presence of water, which is added at 10-50 wt% based on the total amount of the reactants. The reaction takes place at 120-150°C to form an aqueous solution of nylon salt. The solution is heated to 200-260°C to remove all the water before it is subjected to final polycondensation under 270-280°C and reduced pressure.

Nylon 66 is directly prepared from ADA and HMDA without forming the aqueous nylon salt (US 5674974, US 5731403). In the process, an acid-rich molten mixture is first prepared in an agitated reactor from solid granular ADA and liquid HMDA. The molten mixture, containing 81 wt% ADA and 19 wt% HMDA, is continuously fed into the top of an 8-stage vertical column reactor. Liquid HMDA or >58 wt% aqueous HMDA solution is fed below the first stage in the top at various stages 2 through 8 in the reactor. The reactor is equipped with internals, such as perforated plates, coils, and agitators, which provide effective contact of countercurrently flowing diamine stream with a molten acid-rich stream. The resulting polymer has a number average MW of 10500-11000. The loss of diamine through the polymerization reactor is reported less than 100 ppm per part of polymer. Nylon 66 can also be prepared by first reacting melted HMDA with dimethyl adipate at 50°C in the presence of Na-methylate or alkali metal aryloxide (US 5686556). The resulting ester monoamide precipitates during the reaction; it is washed with water, and heated at reflux for 1 hour at 200-270°C to carry out oligomerization with releasing methanol formed during the reaction. The resulting oligomers are further polymerized at 270°C to produce nylon 66.

Nylon resins for injection molding require characteristic of high flow or low melt viscosity. It has been reported that the melt viscosity of nylon resin is improved dramatically by unbalancing the acid and amine end groups. The ratio of end groups, i.e. the number of end groups in excess (either acid end groups or amine end groups) divided by the number of end groups not in excess, is at least 2:1 (US 5824763).

The production of nylon 66 with high MW is achieved by solid-phase polymerization. In US 5955569, moist polyamide pellets prepared from aqueous AH solution is treated countercurrently with nitrogen gas having low dew point in vertical solid-phase polymerization reactor in the presence of a phosphorus-containing catalyst, such as 2(2'-pyridyl)ethyl phosphonic acid. The catalyst is impregnated to the AH salt in the early stage of operation. Although the presence of water in the pellets deactivate the catalyst, the use of low dew point gas provides a driving force, which diffuses the moisture from the interior to the surfaces of the polyamide pellets and evaporates the water from the surfaces. In US 5140098, a linear high MW nylon 66 is prepared by solid-phase polymerization by mixing molten prepolymer with ADA by a weight ratio of 100:0.4-0.8 at 282°C for 2 minutes and pelletized. The resulting granules are subjected solid-phase polycondensation at 180-190°C for 8 hours with superheated steam, which flows countercurrently upward.

The production of nylon 66 from ADN and HMDA through hydrolysis by two-step process was first developed in the 1980s without significant commercial success mainly due to the formation of bis(hexamethylene)triamine (BHMT) in > 1400 ppm levels. The process was operated at a high temperature and high pressure under which dimerization of HMDA is highly promoted. BHMT serves as a crosslinker for the linear polyamide chain, resulting in a high gel content, which leads to significant quality deterioration in the final product. Recently, the process has been modified by allowing full hydrolysis of ADN in the first step with up to 95% of ADN converted to ADA in the presence of phosphorous acid and Ca-hypophosphite as a cocatalyst. The hydrolysate is then polymerized with HMDA in the second step. The BHMT levels were reduced to less than 600 ppm, but the amount of catalyst is high at 1.4 wt% of ADN. It is reported that the amount of the catalyst is reduced to less than 0.1 wt% in US 6084056, but the hydrolysate comprises a mixture of adipamide, adipamic acid, 5-cyanovaleramide, adipic acid, and 5-cyanovaleric acid. In US 6075117, ADN is hydrolyzed with water in the presence of ADA at the amount of 15-20 wt% based on the amount of ADN.

Technology for Reclaim of Nylon Wastes

Polycondensation-polymer wastes, including those from nylon 6 and nylon 66, have been widely disposed of in landfills. However, as landfill areas reach their capacity, disposal of these wastes is becoming increasingly costly. Reclaim of polymer wastes has then become a logical approach. It is well known that polycondensation polymers from polymer processing or post-consumer waste can be depolymerized to some or all of the backbone monomers.

The majority of carpets marketed in the United States and Western Europe comprise a face fiber and a backing material, generally polypropylene fabric, which is held together with a SBR latex adhesive. A variety of inorganic fillers, such as calcium carbonate, clay or hydrated alumina, are also added. The face fiber is nylon 6, nylon 66 or polyester fibers. Several approaches have been considered in the industry to reclaim monomers from the face fibers. In general, the waste carpet is shredded and screened to separate adhesive material. If necessary, the particles are further subjected to size reduction by a hammer mill to remove additional residual adhesive material (US 5948908, US 5932724, US 5929234, US 5869654, US 5722603, US 5681952, US 5656757).

The shredded and screened carpet waste is extracted with water. A surfactant and/or caustic soda may be added during the washing to enhance the removal of other additives, such as oils dyes and stabilizers, and to reduce the bonding strength between the face fiber and the backing materials (US 5722603, US 5457197). The washed carpet waste containing mainly the fiber is depolymerized at 300-340°C with superheated steam in the presence of phosphoric acid (US 5990306, US 5722603, US 5457197, US 5495015). In US 5294707, Nylon 6 is semi-continuously depolymerized with superheated steam in the presence of phosphoric acid as a catalyst. The depolymerization is carried out to a relatively low degree of conversion before recharging the depolymerization reactor with a new batch of nylon 6 waste. For catalysts which are polymerizable, such as ortho-phosphoric acid and p-toluenesulfonic acid, the degree of conversion prior to recharge of nylon waste is preferably 40 to 85 %, while for non-polymerizable catalysts, such as boric acid and 4-sulfoisophthalic acid, the degree of conversion is 75 to 90 %.

Alternatively, the shredded carpet waste is melted in an extruder, and then subjected to hydrolytic depolymerization with water at 295°C (US 5646191, US 5656757). In case of nylon 6 waste, CAPM is recovered through depolymerization requires repeated distillation to achieve desired purity for CAPM to be able recycled to nylon 6 production.

In US 5468900, wastes of nylon 6 and/or nylon 66 are depolymerized in the presence of an aliphatic acid, such as acetic acid or propionic acid and the depolymerized products are further

converted to adipic acid by oxidation. At least one mole of the aliphatic acid is used for every mole of repeat unit of the polymer during the depolymerization of nylon 6. For nylon 66 waste, at least two moles of the aliphatic acid are used for every mole of repeat unit of the polymer. The depolymerization products are 6-acetoamidohexanoic acid in the nylon 6 case, and adipic acid and N,N'-hexamethylene bisalkylamide in the nylon 66 case. These depolymerization products are oxidized either chemically or electrochemically to adipic acid.

The presence of polypropylene fabric, SBR latex and fillers in the backing materials may interfere substantially during the depolymerization process. Separation of these materials involves an initial separation process using a shearing device or serrated rolls. Since the post-consumer carpets come in different shapes and sizes, this makes the separation process difficult to recover most of face fibers from the carpet waste. In US 5722603, the backing materials are separated by dry screen separation after initial shredding operation. A second size reduction by a hammer mill are used to remove additional adhesive material before water washing. After washing the mixture is subjected to a fluidic separation through a series of hydrocyclones to separate the face fiber from the backing materials.

Several recent patents are reported to depolymerize nylon 6 scraps with superheated steam without catalysts (US 5990306, US 5948908, US 5932724, US 5869654, US 5681952, US 5656757, US 5495015, US 5457197). An important benefit of this non-catalyst process is that pre-separation of the non-nylon components in the scraps, such as calcium carbonate, would not be necessary. These components would, otherwise, neutralize the acidic catalyst during depolymerization reaction. The depolymerization temperature, in this case, ranges from 300 to 340°C.

5 ECONOMICS FOR CAPROLACTAM AND NYLON 6

INTRODUCTION

In this section we will provide economics for the production of CAPM by four commercially available processes and those for the production of nylon 6 by a widely used polymerization process.

AVAILABLE COMMERCIAL CAPM PROCESSES

At present, most of the CAPM is commercially prepared via cyclohexanone, which is derived from cyclohexane by oxidation or from phenol by hydrogenation. The cyclohexanone is then converted to cyclohexanone oxime by one of the following two approaches:

- The hydroxylamine phosphate (HPO) process, which uses phosphoric acid as hydroxylamine carrier, produces less amount of ammonium sulfate than the Raschig process.
- The nitric oxide reduction process, which uses hydroxylammonium-ammonium sulfate as hydroxylamine carrier.

A third route, the conventional Raschig process, is no longer used in major production region because the process produces a large amount of ammonium sulfate by-product, which causes troublesome problems for the producers to deposit the material.

Recently, two butadiene-based CAPM processes have been developed; one jointly developed by DSM and DuPont, and the other by BASF and DuPont. They are respectively

- CAPM from butadiene via methyl 6-aminocaproate by carboalkoxylation, hydroformylation and reductive ammoniation followed by cyclization
- CAPM from butadiene via 6-aminocapronitrile by hydrocyanation and partial hydrogenation followed by cyclization

CAPM FROM PHENOL BY HPO PROCESS

Process Description

Figure 5.1 (foldout at end of report) presents the flow diagram for the HPO process, and the utilities summary and major equipment list are given in Table 5.1 and 5.2, respectively. The following is a brief description of the process.

In this process, phenol is pretreated with polyethyleneimine to remove acetol, and distilled. It is then hydrogenated at 10 atm and 173-156°C in the presence of Na-promoted Pd-on-C. Crude cyclohexanone product is purified by distillation. Meantime, ammonia is oxidized to nitrogen oxides. The oxides are converted to ammonium nitrate, which is hydrogenated to hydroxylammonium phosphate (HAP) with the aid of a Pd-on-C catalyst promoted with Pt and GeO₂ in the presence of a buffered monoammonium phosphate/phosphoric acid solution. This solution is circulated between the hydroxylammonium salt synthesis zone and the downstream cyclohexanone oxime synthesis zone without generating (NH₄)₂SO₄. Phosphoric acid consumed

during HAP formation is regenerated in the oximation section. HAP and cyclohexanone undergo oximation at 70°C to form cyclohexanone oxime. The oxime, which is purified by distillation, undergoes Beckmann rearrangement by treatment with oleum to form a caprolactam-sulfuric acid mass. The mass is neutralized and diluted with aqueous ammonia to yield caprolactam and ammonium sulfate. The crude caprolactam is purified by benzene extraction, ion exchange, and hydrogen treatment in the presence of Raney nickel catalyst. It is then subjected to evaporation, caustic soda treatment, further evaporation, and distillation. Purified caprolactam is stored as a molten product. Ammonium sulfate, recovered in the extraction, is purified by crystallization, dried, and bagged or stored in bulk. Product yield on phenol is 94.2%. The phenol-based process is used worldwide and is widely licensed by Stamicarbon.

Economics

Capital investment summary for this process is given in Table 5.3, and those for operation sections are listed in Table 5.4. At a capacity of 309 million lb/yr (140,000 t/yr), the process requires \$207.4 million for the battery limits and \$350.2 million for total fixed capital.

The production costs are summarized in Table 5.5. With a unit price of phenol at 32¢/lb, the cash cost and the plant gate cost for CAPM are estimated at 64.6 ¢/lb and 76 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 113.4 ¢/lb.

Table 5.1
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

UTILITIES SUMMARY

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

UNITS		BATTERY LIMITS	SECTION	SECTION	SECTION	SECTION	SECTION	SECTION
		TOTAL	100	200	300	400	500	600
AVERAGE CONSUMPTIONS								
COOLING WATER	GPM	50,100	5,900	21,000	8,200	--	5,800	9,200
PROCESS WATER	GPM	249	--	6	220	23	--	--
ELECTRICITY	KW	9,871	680	7,600	240	300	390	660
NATURAL GAS	MM BTU/HR	0	--	0	--	--	--	--
INERT GAS, LOW P	M SCF/HR	47	47	--	--	--	--	--
STEAM, 50 PSIG	M LB/HR	109	6	43	--	--	60	--
STEAM, 150 PSIG	M LB/HR	417	32	180	--	--	86	120
STEAM, 300 PSIG	M LB/HR	2	--	2	--	--	--	--
STEAM, 600 PSIG	M LB/HR	18	18	--	--	--	--	--
STEAM, 300 PSIG	M LB/HR	-43	--	-43	--	--	--	--
REFRIGERATION, 40°F	TONS	6,900	--	6,900	--	--	--	--

Table 5.2
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101-105	HYDROGENATORS	5,000 GAL EA	SHELL: C.S. AGITATOR: 304 SS	EACH JACKETED AND EQUIPPED WITH 50 HP TURBINE AGITATOR
R-201	AMMONIA OXIDIZER	16,000 GAL	CLADDING: 316 SS	
R-202A,B	NITRATE HYDROGENATORS	16,000 GAL EA	CLADDING: 316 SS	EACH EQUIPPED WITH 160 HP TURBINE AGITATOR AND 5800 SQFT HEAT EXCHANGER
R-203	METHANIZER	DIA: 3 FT HEIGHT: 19 FT T-T	SHELL: C.S. PACKING: NI-CATALYST	12 FT OF 1/8 IN NICKEL-BASED CATALYST
R-204A,B	MAIN OXIMATORS	32,500 GAL EA	CLADDING: 316 SS AGITATOR: 304 SS	EACH JACKETED AND EQUIPPED WITH 435 HP TURBINE AGITATOR
R-205	POST OXIMATOR	20,000 GAL	CLADDING: 316 SS	WITH 260 HP TURBINE AGITATOR
R-301A,B	REARRANGEMENT REACTORS	36,200 GAL EA	SHELL: C.S.	EACH EQUIPPED WITH SPECIAL MIXING DEVICE AND EXTERNAL CIRCULATION LOOP
R-501	HYDROGENATOR	10,500 GAL	CLADDING: 316 SS	WITH 70 HP TURBINE AGITATOR
COLUMNS				
C-101	PHENOL COLUMN	5.3 FT DIA 30 FT	CLADDING: 316 SS TRAYS: 316 SS	10 VALVE TRAYS, 24 INCH SPACING
C-102	CYCLOHEXANONE COLUMN	10.5 FT DIA 109 FT	CLADDING: 316 SS TRAYS: 316 SS	33 VALVE TRAYS, 36 INCH SPACING
C-103	HEAVY ENDS COLUMN	6.6 FT DIA 60 FT	CLADDING: 316 SS TRAYS: 316 SS	25 VALVE TRAYS, 24 INCH SPACING
C-201	NITROGEN OXIDE ABSORB	5.5 FT DIA 45 FT	CLADDING: 316 SS PACKING: 316 SS	32 FT OF 1 INCH RING PACKING
C-202	DECOMPOSER	4 FT DIA 30 FT	CLADDING: 316 SS PACKING: 316 SS	20 FT OF 1 INCH RING PACKING
C-203	EXTRACTOR	11 FT DIA 18 FT	CLADDING: 316 SS TRAYS: 316 SS	8 SIEVE TRAYS, 24 INCH SPACING 8 ROTARY DISCS AND 88 HP DRIVE
C-204	STRIPPER	10 FT DIA 55 FT	CLADDING: 316 SS TRAYS: 316 SS	15 SIEVE TRAYS, 36 INCH SPACING
C-205	TOLUENE COLUMN	14 FT DIA 34 FT	CLADDING: 316 SS TRAYS: 316 SS	8 SIEVE TRAYS, 36 INCH SPACING
C-206	OXIME RECTIFIER	14 FT DIA 50 FT	CLADDING: 316 SS TRAYS: 316 SS	20 SIEVE TRAYS, 24 INCH SPACING
C-401	SULFATE REMOVAL COLUMN	6.3 FT DIA 46 FT	CLADDING: 316 SS TRAYS: 316 SS	17 VALVE TRAYS, 24 INCH SPACING WITH 17 ROTARY DISCS AND 88 HP DRIVE
C-402	BENZENE EXTRACTOR	5.5 FT DIA 46 FT	CLADDING: 316 SS TRAYS: 316 SS	17 VALVE TRAYS, 24 INCH SPACING WITH 17 ROTARY DISCS AND 65 HP DRIVE
C-403	WATER WASH COLUMN	5.5 FT DIA 46 FT	CLADDING: 316 SS PACKING: PORCELAIN	36 FT OF 1 INCH RING PACKING
C-404	SECONDARY BENZENE COLN	4 FT DIA 46 FT	SHELL: 316 SS PACKING: PORCELAIN	36 FT OF 1 INCH RING PACKING
C-405	WATER EXTRACTION COLN	6.4 FT DIA 46 FT	CLADDING: 316 SS TRAYS: 316 SS	17 VALVE TRAYS, 24 INCH SPACING WITH 17 ROTARY DISCS, 90 HP DRIVE
C-501A,B	ION EXCHANGERS	6.8 FT DIA 20 FT	CLADDING: 316 SS PACKING: ALUMINA	14 FT OF PACKING
C-502	LIGHT ENDS COLUMN	2 FT DIA 40 FT	SHELL: 316 SS PACKING: 316 SS	30 FT OF 1 INCH RING PACKING
C-503A-C	PRODUCT COLUMNS	10 FT DIA 20 FT	CLADDING: 316 SS PACKING: 316 SS	10 FT OF 1 INCH RING PACKING
C-504	HEAVY ENDS COLUMN	7.7 FT DIA 20 FT	CLADDING: 316 SS PACKING: 316 SS	10 FT OF 1 INCH RING PACKING

Table 5.2 (Continued)
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
COMPRESSORS				
K-101	COMPRESSOR	366 BHP	316 SS	
K-201	COMPRESSOR	6,700 BHP	C.S.	WITH A 2370 SQFT INTERCOOLER
K-202	COMPRESSOR	165 BHP	316 SS	
K-501	COMPRESSOR	14 BHP	316 SS	
HEAT EXCHANGERS				
E-101	HEATER	440 SQ FT	SHELL: C.S. TUBES: 316 SS	
E-102	CONDENSER	3.75 MMBTU/HR		
E-103	REBOILER	600 SQ FT	SHELL: C.S.	
E-104	CONDENSER	12.33 MMBTU/HR	TUBES: 316 SS	
E-105	CONDENSER	3,130 SQ FT	SHELL: C.S.	
E-106	CONDENSER	12.51 MMBTU/HR	TUBES: 316 SS	
E-107	CONDENSER	140 SQ FT	SHELL: C.S.	
E-108	CONDENSER	1.77 MMBTU/HR	TUBES: 316 SS	
E-109	COOLER	1.77 MMBTU/HR	SHELL: C.S.	
E-110	CONDENSER	55 SQ FT	TUBES: 316 SS	
E-111	CONDENSER	1.53 MMBTU/HR	SHELL: C.S.	
E-112	CONDENSER	1,800 SQ FT	TUBES: 316 SS	
E-113	REBOILER	21.17 MMBTU/HR	SHELL: C.S.	
E-114	CONDENSER	2,300 SQ FT	TUBES: 316 SS	
E-201	AMMONIA EVAPORATOR	20.66 MMBTU/HR	SHELL: C.S.	
E-202	AMMONIA SUPERHEATER	460 SQ FT	TUBES: 316 SS	
E-203	AIR PREHEATER	3.79 MMBTU/HR	SHELL: C.S.	
E-204	HEAT EXCHANGER	900 SQ FT	TUBES: 316 SS	
E-205	HEAT EXCHANGER	3.8 MMBTU/HR	SHELL: C.S.	
E-206	COOLER	1,800 SQ FT	TUBES: 316 SS	
E-207	HEATER	4.6 MMBTU/HR	SHELL: C.S.	
E-208	COOLER	200 SQ FT	TUBES: 316 SS	
E-209	CONDENSER	1.3 MMBTU/HR	SHELL: C.S.	
E-210	REBOILER	1,660 SQ FT	TUBES: 316 SS	
E-211	COOLER	3.4 MMBTU/HR	SHELL: C.S.	
E-212	CONDENSER	2,630 SQ FT	TUBES: 316 SS	
		8.6 MMBTU/HR	SHELL: C.S.	
		2,250 SQ FT	TUBES: 316 SS	
		16.6 MMBTU/HR	SHELL: C.S.	
		130 SQ FT	TUBES: 316 SS	
		0.33 MMBTU/HR	SHELL: C.S.	
		100 SQ FT	TUBES: 316 SS	
		0.6 MMBTU/HR	SHELL: C.S.	
		2,570 SQ FT	TUBES: 316 SS	
		134.3 MMBTU/HR	SHELL: C.S.	
		6,460 SQ FT	TUBES: 316 SS	
		50 MMBTU/HR	SHELL: C.S.	
		11,030 SQ FT	TUBES: 316 SS	
		38.6 MMBTU/HR	SHELL: C.S.	
			TUBES: 316 SS	

Table 5.2 (Continued)
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONCLUDED)				
E-213	REBOILER	5,780 SQ FT 39.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-214	CONDENSER	1,640 SQ FT 12.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-215	REBOILER	2,620 SQ FT 14.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-301A,B	COOLERS	2,560 SQ FT EA 17.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-302	COOLER	8,070 SQ FT 46.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-501	CONDENSER	3,940 SQ FT 35.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-502A,B	CONDENSERS	130 SQ FT EA 4.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-503	CONDENSER	25 SQ FT 0.2 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-504A-C	CONDENSERS	420 SQ FT EA 3.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-505	CONDENSER	220 SQ FT 2 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-601A-C	CONDENSERS	8,680 SQ FT EA 30.8 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
DIRECT-FIRED HEATERS				
H-201	DOWTHERM HEATER	0.33 MMBTU/HR	C.S.	
TANKS				
T-101	PHENOL FEED TANK	104,000 GAL	NI-LINED	WITH HEATING COILS
T-102	PHENOL SURGE TANK	43,000 GAL	NI-LINED	WITH HEATING COILS
T-103	CR. CYCLOHEXANONE TANK	62,000 GAL	316 SS	
T-104	CYCLOHEXANONE TANK	49,000 GAL	316 SS	
T-151	PHENOL STORAGE	520,000 GAL	NI-LINED	WITH HEATING COILS
T-201	HYDROXYL AMMONIUM TK	550,000 GAL	316 SS	
T-202	TOLUENE TANK	243,000 GAL	C.S.	
T-251A,B	AMMONIA STORAGE	252,000 GAL EA	NI-LINED	NOT SHOWN IN FLOW DIAGRAM
T-252	WASTE WATER TANK	353,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-301	OLEUM TANK	85,600 GAL	RUBBER LINED	
T-302	AMMONIA WATER	176,000 GAL	C.S.	
T-303	CRUDE CAPM TANK	68,700 GAL	316 SS	
T-351	OLEUM STORAGE	428,000 GAL	RUBBER LINED	NOT SHOWN IN FLOW DIAGRAM
T-401	LACTAM-BENZENE TANK	297,400 GAL	316 SS	
T-501	CAPM SURGE TANK	183,800 GAL	316 SS	
T-502	CAUSTIC SODA TANK	50 GAL	316 SS	
T-503	CRUDE CAPM TANK	71,600 GAL	316 SS	WITH HEATING COILS
T-504	PURIFIED CAPM TANK	125,000 GAL	316 SS	WITH HEATING COILS
T-551A,B	CAPM STORAGE	320,000 GAL EA	316 SS	NOT SHOWN IN FLOW DIAGRAM
T-601	AMMONIUM SULFATE TANK	186,000 GAL	C.S.	WITH HEATING COILS
T-602	MOTHER LIQUOR TANK	37,700 GAL	304 SS	WITH HEATING COILS

Table 5.2 (Continued)
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
PRESSURE VESSELS				
V-101A,B	MIXING VESSELS	1,170 GAL EA	316 SS	EACH EQUIPPED WITH 15 HP TURBINE AGITATOR
V-102	TREATMENT VESSEL	5,200 GAL	C.S.	WITH 50 HP TURBINE AGITATOR
V-103	REFLUX DRUM	1,500 GAL	316 SS	
V-104	CATALYST VESSEL	600 GAL	316 SS	WITH 8 HP TURBINE AGITATOR
V-105	REFLUX DRUM	4,500 GAL	304 SS CLAD	
V-106	REFLUX DRUM	1,000 GAL	316 SS	
V-201	COPRECIPITATION VESSEL	29,600 GAL	316 SS CLAD	WITH 250 HP TURBINE AGITATOR
V-202A,B	REAGENT VESSELS	1,850 GAL EA	316 SS	EACH EQUIPPED WITH 18 HP TRUBINE AGITATOR
V-203	HIGH PRESSURE SEPARATR	20,500 GAL	316 SS CLAD	
V-204	DECANTER	32,500 GAL	316 SS CLAD	
V-205	REFLUX DRUM	3,770 GAL	C.S.	
V-206	DECANTER	17,540 GAL	316 SS CLAD	
V-207	REFLUX DRUM	11,060 GAL	C.S.	
V-208	REFLUX DRUM	3,100 GAL	C.S.	
V-301	OXIME SURGE VESSEL	54,950 GAL	316 SS CLAD	
V-302	NEUTRALIZATION VESSEL	4,780 GAL	316 SS CLAD	WITH 48 HP TURBINE AGITATOR
V-303	DECANTER	13,080 GAL	316 SS CLAD	
V-401	DECANTER	5,900 GAL	316 SS CLAD	
V-402	PH ADJUSTMENT VESSEL	5,170 GAL	316 SS CLAD	WITH 45 HP TURBINE AGITATOR
V-403	DECANTER	3,940 GAL	316 SS CLAD	
V-501A,B	CATALYST VESSELS	300 GAL EA	316 SS	EACH EQUIPPED WITH 4 HP TURBINE AGITATOR
V-502A,B	RECEIVERS	190 GAL EA	316 SS	
V-503	REFLUX DRUM	45 GAL	316 SS	
V-504A-C	REFLUX DRUMS	650 GAL EA	316 SS	
V-505	REFLUX DRUM	380 GAL	316 SS	
V-601A-C	CONDENSATE RECEIVERS	1,350 GAL EA	C.S.	
MISCELLANEOUS EQUIPMENT				
M-101	WEIGH SCALE	100 LB DIAL	C.S.	
M-102	FILTER	CARTRIDGE	C.S.	
M-103	VACUUM SYSTEM	100-200 MMHG	C.S.	NOT SHOWN IN FLOW DIAGRAM
M-201	AIR FILTER	136200 LB/HR	316 SS	
M-202	WEIGH SCALE	100 LB DIAL	C.S.	
M-203	FILTER	CARTRIDGE	316 SS	
M-204	FILTER	CARTRIDGE	316 SS	
M-205	VACUUM SYSTEM	60-150 MMHG	C.S.	NOT SHOWN IN FLOW DIAGRAM
M-301A,B	STATIC MIXERS	1450 GPM EA	316 SS	
M-401	STATIC MIXER	440 GPM	316 SS	
M-402	VACUUM SYSTEM	100 MMHG	C.S.	NOT SHOWN IN FLOW DIAGRAM
M-501	WEIGH SCALE	100 LB DIAL	C.S.	
M-502	FLITER	CARTRIDGE	316 SS	
M-503	VACUUM SYSTEM	5-10 MMHG	C.S.	NOT SHOWN IN FLOW DIAGRAM
M-601	VACUUM SYSTEM	150 MMHG	C.S.	NOT SHOWN IN FLOW DIAGRAM
SPECIAL EQUIPMENT				
S-101	HEAVY ENDS SEPARATOR	68 SQFT	C.S.	THIN FILM EVAPORATOR WITH 12 HP DRIVE
S-102	CENTRIFUGE	18 IN DIA	316 SS	WITH 15 HP DRIVE
S-501A-C	EVAPORATORS	1800 SQFT EA	316 SS	TRIPLE EFFECT EVAPORATORS
S-504A,B	EVAPORATORS	445 SQFT EA	316 SS	THIN FILM EVAPORATORS EACH WITH 50 HP DRIVE
S-505	EVAPORATOR	101 SQFT	316 SS	THIN FILM EVAPORATOR WITH 20 HP DRIVE
S-506A-C	EVAPORATORS	440 SQFT EA	316 SS	THIN FILM EVAPORATORS EACH WITH 50 HP DRIVE
S-507	EVAPORATOR	268 SQFT	316 SS	THIN FILM EVAPORATOR WITH 30 HP DRIVE
S-601A-C	CRYSTALLIZERS	260 TONS/DAY EA	316 SS	EACH EQUIPPED WITH 21 HP DRIVE
S-602A-C	THICKENERS	260 TONS/DAY EA	316 SS	EACH EQUIPPED WITH 80 PH DRIVE
S-603A-C	CENTRIFUGES	13 TONS/HR EA	316 SS	

Table 5.2 (Concluded)
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
SPECIAL EQUIPMENT (CONCLUDED)				
S-604A-C	ROTARY DRYERS	12 FT X 55 FT EA	C.S.	EACH EQUIPPED WITH 102 HP DRIVE
S-605A-C	BUCKET ELEVATORS	12 TONS/HR EA	316 SS	EACH EQUIPPED WITH 3 HP DRIVE
S-606A-C	HOPPERS	6 FT X 20 FT EA	316 SS	
S-607A-C	SIFTERS	6 SQFT EA	316 SS	SINGLE DECK
S-608A-C	CRUSHERS	12 TONS/HR EA	316 SS	EACH EQUIPPED WITH 9 HP DRIVE
S-609A-C	BAGGING UNITS	7 BAGS/MIN EA	316 SS	
PUMPS				
SECTION	OPERATING	SPARES	OPERATING BHP	
100	10	10	85	
200	21	19	434	
300	7	7	236	
400	6	6	78	
500	12	10	82	
600	12	8	118	

Table 5.3
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

TOTAL CAPITAL INVESTMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	5,343	0.76	0.70
COLUMNS	5,046	0.82	0.69
VESSELS & TANKS	7,629	0.66	0.57
HEAT EXCHANGERS	5,347	0.88	0.81
FURNACES	22	0.79	0.74
COMPRESSORS	5,128	0.88	0.76
SPECIAL EQUIPMENT	15,761	0.69	0.67
MISCELLANEOUS EQUIPMENT	463	0.59	0.59
PUMPS	1,897	0.54	0.43
-----	-----	-----	-----
TOTAL	46,636	0.75	0.67
DIRECT INSTALLATION COSTS	68,241	0.46	0.37
INDIRECT COSTS	35,981	0.49	0.40
UNSCHEDULED EQUIPMENT, 10%	15,086	0.56	0.47
-----	-----	-----	-----
BATTERY LIMITS, INSTALLED	165,945	0.56	0.47
CONTINGENCY, 25%	41,486	0.56	0.47
-----	-----	-----	-----
BATTERY LIMITS INVESTMENT	207,431	0.56	0.47
OFF-SITES, INSTALLED			
CLARIFIED WATER	1,826	0.74	0.74
COOLING WATER	9,668	0.95	0.92
PROCESS WATER	1,064	0.62	0.62
BOILER FEED WATER	2,670	0.44	0.39
STEAM	14,596	0.76	0.66
REFRIGERATION	12,907	0.95	0.90
INERT GAS	358	0.95	0.52
TANKAGE	5,124	0.66	0.65
WAREHOUSE FACILITIES	3,744	0.60	0.60
-----	-----	-----	-----
UTILITIES & STORAGE	51,958	0.81	0.74
GENERAL SERVICE FACILITIES	51,878	0.62	0.52
WASTE TREATMENT	10,372	0.56	0.47
-----	-----	-----	-----
TOTAL	114,208	0.70	0.61
CONTINGENCY, 25%	28,552	0.70	0.61
-----	-----	-----	-----
OFF-SITES INVESTMENT	142,760	0.70	0.61
TOTAL FIXED CAPITAL	350,191	0.62	0.52

Table 5.4
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

CAPITAL INVESTMENT BY SECTION

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
CAPROLACTAM
AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	PHENOL HYDROGENATION			CYCLOHEXANONE OXIMATION			OXIME REARRANGEMENT		
	CAPACITY EXPONENT			CAPACITY EXPONENT			CAPACITY EXPONENT		
	COST (\$1,000)	UP	DOWN	COST (\$1,000)	UP	DOWN	COST (\$1,000)	UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	1,464	0.71	0.70	3,267	0.79	0.71	377	0.70	0.70
COLUMNS	637	0.83	0.50	1,963	0.85	0.72	--	--	--
VESSELS & TANKS	1,926	0.63	0.48	2,035	0.67	0.64	954	0.71	0.62
HEAT EXCHANGERS	839	0.85	0.81	2,806	0.89	0.83	841	0.90	0.83
FURNACES	--	--	--	22	0.79	0.74	--	--	--
COMPRESSORS	1,084	0.76	0.76	3,952	0.92	0.76	--	--	--
SPECIAL EQUIPMENT	258	0.70	0.68	--	--	--	--	--	--
MISCELLANEOUS EQUIPMENT	78	0.58	0.58	140	0.61	0.61	22	0.58	0.58
PUMPS	282	0.37	0.28	678	0.57	0.48	378	0.73	0.57
TOTAL	6,567	0.71	0.61	14,863	0.83	0.73	2,572	0.77	0.69
DIRECT INSTALLATION COSTS	11,198	0.44	0.36	26,544	0.57	0.46	3,191	0.45	0.35
INDIRECT COSTS	5,564	0.46	0.36	12,969	0.58	0.46	1,805	0.52	0.41
UNSCHEDULED EQUIPMENT, 10%	2,333	0.52	0.43	5,438	0.65	0.53	757	0.59	0.47
BATTERY LIMITS INSTALLED	25,662	0.52	0.43	59,815	0.65	0.53	8,325	0.59	0.47
CONTINGENCY, 25%	6,415	0.52	0.43	14,954	0.65	0.53	2,081	0.59	0.47
BATTERY LIMITS INVESTMENT	32,077	0.52	0.43	74,768	0.65	0.53	10,406	0.59	0.47
OFFSITES, INSTALLED									
CLARIFIED WATER	167	0.74	0.74	835	0.74	0.74	353	0.74	0.74
COOLING WATER	966	0.95	0.92	4,905	0.95	0.92	1,342	0.95	0.92
PROCESS WATER	96	0.62	0.62	489	0.62	0.62	134	0.62	0.62
BOILER FEED WATER	816	0.11	0.08	890	0.53	0.51	--	--	--
STEAM	3,648	0.28	0.17	4,549	0.90	0.86	--	--	--
REFRIGERATION	--	--	--	12,907	0.95	0.90	--	--	--
INERT GAS	358	0.95	0.52	--	--	--	--	--	--
TANKAGE	--	--	--	2,429	0.67	0.65	623	0.65	0.65
WAREHOUSE FACILITIES	--	--	--	--	--	--	--	--	--
UTILITIES & STORAGE	6,050	0.46	0.30	27,003	0.89	0.85	2,451	0.83	0.81

Table 5.4 (Concluded)

CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

CAPITAL INVESTMENT BY SECTION

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
CAPROLACTAM
AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	CAPROLACTAM EXTRACTION			CAPROLACTAM PURIFICATION			AMMONIUMSULFATE RECOVERY		
	CAPACITY EXPONENT			CAPACITY EXPONENT			CAPACITY EXPONENT		
	COST (\$1,000)	UP	DOWN	COST (\$1,000)	UP	DOWN	COST (\$1,000)	UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	--	--	--	235	0.68	0.64	--	--	--
COLUMNS	816	0.61	0.49	1,629	0.87	0.84	--	--	--
VESSELS & TANKS	964	0.64	0.63	1,368	0.62	0.59	382	0.77	0.43
HEAT EXCHANGERS	--	--	--	433	0.84	0.80	428	0.95	0.63
FURNACES	--	--	--	--	--	--	--	--	--
COMPRESSORS	--	--	--	92	0.76	0.76	--	--	--
SPECIAL EQUIPMENT	--	--	--	7,729	0.75	0.72	7,774	0.63	0.63
MISCELLANEOUS EQUIPMENT	82	0.55	0.54	121	0.62	0.62	20	0.58	0.49
PUMPS	143	0.53	0.44	267	0.41	0.32	150	0.43	0.33
TOTAL	2,005	0.62	0.56	11,875	0.75	0.71	8,754	0.65	0.61
DIRECT INSTALLATION COSTS	3,444	0.31	0.30	13,576	0.34	0.29	10,289	0.39	0.33
INDIRECT COSTS	1,707	0.34	0.30	7,972	0.45	0.39	5,965	0.43	0.37
UNSCHEDULED EQUIPMENT, 10%	715	0.41	0.37	3,342	0.52	0.45	2,501	0.49	0.43
BATTERY LIMITS INSTALLED	7,870	0.41	0.37	36,765	0.52	0.45	27,508	0.49	0.43
CONTINGENCY, 25%	1,968	0.41	0.37	9,191	0.52	0.45	6,877	0.49	0.43
BATTERY LIMITS INVESTMENT	9,838	0.41	0.37	45,957	0.52	0.45	34,385	0.49	0.43
OFFSITES, INSTALLED									
CLARIFIED WATER	15	0.74	0.74	188	0.74	0.74	269	0.74	0.74
COOLING WATER	--	--	--	949	0.95	0.92	1,506	0.95	0.92
PROCESS WATER	--	--	--	95	0.62	0.62	150	0.62	0.62
BOILER FEED WATER	--	--	--	530	0.58	0.58	435	0.58	0.58
STEAM	--	--	--	3,512	0.90	0.86	2,887	0.90	0.86
REFRIGERATION	--	--	--	--	--	--	--	--	--
INERT GAS	--	--	--	--	--	--	--	--	--
TANKAGE	--	--	--	2,073	0.65	0.65	--	--	--
WAREHOUSE FACILITIES	--	--	--	--	--	--	3,744	0.60	0.60
UTILITIES & STORAGE	15	0.74	0.74	7,346	0.81	0.78	8,991	0.77	0.74

Table 5.5
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
AMMONIA	8.75 ¢/LB	0.65815 LB	5.76
HYDROGEN	0.388 ¢/FT^3	18.8 FT^3	7.29
OLEUM (7%)	4.01 ¢/LB	1.29795 LB	5.20
PHENOL	32 ¢/LB	0.8826 LB	28.24
CATALYSTS AND OTHER CHEM			2.04
GROSS RAW MATERIALS			48.53
BY-PRODUCTS			
AMMONIUM SULFATE	1.9 ¢/LB	-1.778 LB	-3.38
FUEL	2.21 \$/MMBTU	-0.0004 MMBTU	-0.09
TOTAL BY-PRODUCTS			-3.47
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	76.8 GAL	0.57
PROCESS WATER	1.101 \$/MGAL	0.382 GAL	0.04
STEAM, 150 PSIG	4.51 \$/MLB	12.4 LB	5.60
STEAM, 600 PSIG	5.72 \$/MLB	0.45 LB	0.26
ELECTRICITY	4 ¢/KWH	0.252 KWH	0.556 KWH
NATURAL GAS	3.24 \$/MMBTU	11.2 BTU	6.25 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	1.2 SCF	75 LITERS
REFRIGERATION, 40°F	4.99 ¢/TON-HR	0.176 TON-HR	1.37 KWH
TOTAL UTILITIES			8.42

Table 5.5 (Concluded)
CAPROLACTAM FROM PHENOL BY HYDROXYLAMINE PHOSPHATE OXIME PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	154	309#	617
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	149.9	207.4	306.4
OFFSITES	93.4	142.8	232.5
TOTAL FIXED CAPITAL (TFC)	243.4	350.2	538.9
SCALING EXPONENTS	0.52	0.62	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	48.53	48.53	48.53
BY-PRODUCTS	-3.47	-3.47	-3.47
UTILITIES	8.42	8.42	8.42
VARIABLE COSTS	53.48	53.48	53.48
OPERATING LABOR, 15/SHIFT, \$33.58/HOUR	2.86	1.43	0.72
MAINTENANCE LABOR, 3%/YR OF BLI	2.92	2.02	1.49
CONTROL LAB LABOR, 20% OF OPER LABOR	0.57	0.29	0.14
LABOR COSTS	6.35	3.74	2.35
MAINTENANCE MATERIALS, 3%/YR OF BLI	2.92	2.02	1.49
OPERATING SUPPLIES, 10% OF OPER LABOR	0.29	0.14	0.07
TOTAL DIRECT COSTS	63.04	59.38	57.39
PLANT OVERHEAD, 80% OF LABOR COSTS	5.08	2.99	1.88
TAXES AND INSURANCE, 2%/YR OF TFC	3.15	2.27	1.75
PLANT CASH COSTS	71.27	64.64	61.02
DEPRECIATION, 10%/YR OF TFC	15.77	11.35	8.73
PLANT GATE COSTS	87.04	75.99	69.75
G&A, SALES, RESEARCH	9.00	9.00	9.00
NET PRODUCTION COST	96.04	84.99	78.75
ROI BEFORE TAXES, 25%/YR OF TFC	39.44	28.37	21.83
PRODUCT VALUE	135.48	113.36	100.58

* OF CAPROLACTAM

BASE CASE

CAPM FROM CYCLOHEXANE BY NITRIC OXIDE PROCESS

Process Description

Figure 5.2 (foldout at end of report) presents the flow diagram for this process, and the utilities summary and major equipment list are given in Table 5.6 and 5.7, respectively. A brief description of the process is given below.

Liquid cyclohexane undergoes scrubbing and stripping pretreatment to reduce water content. The cyclohexane is then oxidized at 160°C and 10 atm with air. Liquid oxidation product goes to a decomposition column for treatment with aqueous NaOH solution and cobalt sulfate to convert formed cyclohexyl hydroperoxide into cyclohexanol and cyclohexanone. The treated oxidation product is distilled to recover unreacted cyclohexane for recycle. After cyclohexane removal, the oxidation product is saponified with aqueous NaOH solution to remove carboxylic ester impurities as sodium carboxylates. The product, rich in cyclohexanol and cyclohexanone, is washed with dilute aqueous acetic acid and then dehydrated to remove water and cyclohexane. The washed product is finally distilled to yield cyclohexanone. The cyclohexanol is distilled, dehydrogenated to cyclohexanone, and recycled to dehydration.

Ammonia is catalytically oxidized with O₂ in the presence of steam, then hydrogenated using a Pd-on-C catalyst to form hydroxylamine in the form of hydroxylammonium-ammonium sulfate (HAAS) in a buffer solution of ammonium sulfate and ammonium bisulfate. HAAS solution and cyclohexanone are sent to an oximation reactor operating at 90°C and 1 atm. Reactor effluent goes to an after reactor where pH is adjusted with ammonia to drive the oximation reaction to 97% conversion of cyclohexanone. The oxime is reacted with oleum at 80°C in a stirred reactor. Reactor effluent flows to a decanter where cyclohexane solvent is separated from caprolactam-oleum (C-O) mixture. Cyclohexane and about 79% of the C-O mixture are recycled to the reactor. The rest of the C-O mixture is neutralized with aqueous ammonia to liberate caprolactam. The mixture goes to a decanter. The aqueous (NH₄)₂SO₄ layer goes to recovery. Crude caprolactam is extracted with benzene and is purified by distillation. Additional caprolactam is recovered by batch distillation of distillation residue. Purified caprolactam is stored as a molten product. (NH₄)₂SO₄ is purified by crystallization, dried, and bagged or stored.

Economics

Capital investment summary for this process is given in Table 5.8, and those for operation sections are listed in Table 5.9. At a capacity of 309 million lb/yr (140,000 t/yr), the process requires \$205.2 million for the battery limits and \$381.3 million for total fixed capital.

The production costs are summarized in Table 5.10. With a unit price of cyclohexane at 15.62 ¢/lb, the cash cost and the plant gate cost for CAPM are estimated at 49.9 ¢/lb and 62.3¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 102.2 ¢/lb.

Table 5.6
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

UTILITIES SUMMARY							
UNITS	BATTERY LIMITS		SECTION	SECTION	SECTION	SECTION	SECTION
	TOTAL	100	200	300	400	500	
AVERAGE CONSUMPTIONS							
COOLING WATER	GPM	79,100	51,200	2,800	4,300	11,800	9,000
PROCESS WATER	GPM	368	83	65	--	220	--
ELECTRICITY	KW	5,798	4,400	91	57	660	590
NATURAL GAS	MM BTU/HR	14	14	--	--	--	--
INERT GAS, LOW P	M SCF/HR	44	17	12	1	12	2
STEAM, 150 PSIG	M LB/HR	334	160	--	45	29	100
STEAM, 600 PSIG	M LB/HR	449	390	--	--	59	--
STEAM, 10 PSIG	M LB/HR	-46	--	-46	--	--	--
STEAM, 45 PSIG	M LB/HR	-79	-79	--	--	--	--
REFRIGERATION, 40°F	TONS	5,700	--	2,600	--	3,100	--

Table 5.7
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101-104	OXIDATION REACTORS	24,000 GAL EA	CLADDING: 316 SS	EACH JACKETED AND WITH 200 HP TURBINE AGITATOR
R-105	DEHYDROGENATION REACTOR	8,220 GAL	SHELL: 316 SS	785 TUBES OF 2 IN DIAMETER AND 20 FT LONG
R-201	CONVERTER	1,400 GAL	SHELL: 316 SS	PLATINUM-RHODIUM CATALYST WITH PD-AU BACK-UP GAUZE
R-202	HYDROXYLAMINE REACTOR	DIA: 7 FT HEIGHT: 54 FT T-T	CLADDING: HASTELLOY TRAYS: HASTELLOY	75 TUBULAR GRID TRAYS AT 6 IN SPACING AND 4 GRID TRAYS AT 18 IN SPACING
R-203	(NH4)2SO4 DECOMPSOR	DIA: 5 FT HEIGHT: 25 FT T-T	CLADDING: 316 SS PACKING: 316 SS	20 FT OF 1 INCH RING PACKING
R-301	OXIMATION REACTOR	DIA: 6 FT HEIGHT: 64 FT T-T	CLADDING: 316 SS PACKING: 316 SS	54 FT OF 1 INCH RING PACKING
R-302	AFTER REACTOR	2,200 GAL	CLADDING: 316 SS	WITH 20 HP TURBINE AGITATOR
R-401	REARRANGEMENT REACTOR	25,000 GAL	CLADDING: 316 SS	JACKETED AND WITH 250 HP TURBINE AGITATOR
COLUMNS				
C-101	SCRUBBER	DIA: 2.5 FT HEIGHT: 64 FT T-T	SHELL: 304 SS PACKING: 316 SS	50 FT OF 1 INCH RING PACKING
C-102	STRIPPER	DIA: 8 FT HEIGHT: 64 FT T-T	CLADDING: 304 SS TRAYS: 316 SS	26 VALVE TRAYS, 24 INCH SPACING
C-103	DECOMPOSITION COLUMN	DIA: 13 FT HEIGHT: 34 FT T-T	CLADDING: 316 SS DISCS: 316 SS	WITH 8 ROTARY DISCS, 120 HP DRIVE
C-104A-D	CYCLOHEXANE COLUMNS	DIA: 16 FT EA HEIGHT: 85 FT T-T	CLADDING: 304 SS TRAYS: 304 SS	EACH WITH 25 VALVE TRAYS, 36 INCH SPACING
C-105	SAPONIFICATION COLUMN	DIA: 3 FT HEIGHT: 40 FT T-T	CLADDING: 316 SS TRAYS: 316 SS	15 SIEVE TRAYS, 24 INCH SPACING
C-106	WASHING COLUMN	DIA: 3.5 FT HEIGHT: 28 FT T-T	CLADDING: 316 SS PACKING: 316 SS	24 FT OF 1 INCH RING PACKING
C-107	DEHYDRATION COLUMN	DIA: 8.5 FT HEIGHT: 34 FT T-T	CLADDING: 304 SS TRAYS: 316 SS	12 VALVE TRAYS, 24 INCH SPACING
C-108A,B	LIGHT ENDS COLUMNS	DIA: 9 FT EA HEIGHT: 200 FT T-T	CLADDING: 304 SS TRAYS: 316 SS	EACH WITH 95 SIEVE TRAYS, 24 INCH SPACING
C-109A,B	CYCLOHEXANONE COLUMNS	DIA: 14 FT EA HEIGHT: 130 FT T-T	CLADDING: 304 SS TRAYS: 316 SS	EACH WITH 60 SIEVE TRAYS, 24 INCH SPACING
C-110A,B	CYCLOHEXANOL COLUMN	DIA: 9 FT EA HEIGHT: 68 FT T-T	CLADDING: 304 SS TRAYS: 316 SS	EACH WITH 29 SIEVE TRAYS, 24 INCH SPACING
C-201	ABSORBER	DIA: 3.5 FT HEIGHT: 18 FT T-T	CLADDING: 304 SS PACKING: 316 SS	10 FT OF 1 INCH RING PACKING
C-202A,B	CARBON TREATMENT COLNS	DIA: 7.5 FT EA HEIGHT: 12 FT T-T	CLADDING: 316 SS PACKING: ACTIVATED CARBON	EACH WITH 8 FT OF PACKING
C-301A,B	CYCLOHEXANONE STRIPPER	DIA: 10 FT EA HEIGHT: 82 FT T-T	CLADDING: 316 SS TRAYS: 316 SS	EACH WITH 36 VALVE TRAYS, 24 INCH SPACING
C-302	EXTRACTION COLUMN	DIA: 6 FT HEIGHT: 30 FT T-T	CLADDING: 316 SS TRAYS: 316 SS	12 SIEVE TRAYS, 24 INCH SPACING WITH 12 ROTARY DISCS, 170 HP DRIVE
C-303	OXIMATION REACTOR	DIA: 6 FT HEIGHT: 64 FT T-T	CLADDING: 316 SS PACKING: 316 SS	54 FT OF 1 INCH RING PACKING
C-401	BENZENE EXTRACTION CLN	DIA: 6 FT HEIGHT: 80 FT T-T	CLADDING: 316 SS TRAYS: 316 SS	35 VALVE TRAYS, 24 INCH SPACING WITH 35 ROTARY DISCS, 170 HP DRIVE
C-402	AMMONIUM SULFATE REC	DIA: 6 FT HEIGHT: 28 FT T-T	CLADDING: 316 SS PACKING: 316 SS	18 FT OF 1 INCH RING PACKING
C-403A,B	BENZENE COLUMNS	DIA: 11 FT EA HEIGHT: 39 FT T-T	CLADDING: 316 SS TRAYS: 316 SS	EACH WITH 9 VALVE TRAYS, 36 INCH SPACING
C-404A,B	CAPROLACTAM COLUMNS	DIA: 12.5 FT EA HEIGHT: 48 FT T-T	CLADDING: 316 SS TRAYS: 316 SS	EACH WITH 18 SIEVE TRAYS, 24 INCH SPACING

Table 5.7 (Continued)
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
COMPRESSORS				
K-101A,B	AIR COMPRESSOR	3,860 BHP	C.S.	
HEAT EXCHANGERS				
E-101	CONDENSER	2,000 SQ FT 5.2 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-102	PREHEATER	7,400 SQ FT 55 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-103	COOLER	4,000 SQ FT 53.1 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-104A-D	CONDENSERS	12,000 SQ FT 79.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-105A-D	REBOILERS	6,100 SQ FT 83 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-106	COOLER	80 SQ FT 1.11 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-107	COOLER	350 SQ FT 3.32 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-108	CONDENSER	1,320 SQ FT 5.1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-109	REBOLIER	5,300 SQ FT 10.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-110A,B	CONDENSERS	900 SQ FT 10.8 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-111A,B	REBOILERS	1,570 SQ FT 10.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-112A,B	CONDENSERS	2,330 SQ FT EA 13.6 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-113A,B	REBOILERS	1,000 SQ FT EA 13.9 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-114A,B	CONDENSERS	750 SQ FT EA 5.75 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-115A,B	REBOILERS	900 SQ FT EA 6.04 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-116	VAPORIZER	1,000 SQ FT 8.2 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-117	CONDENSER	1,700 SQ FT 11.7 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-201	AMMONIA PREHEATER	60 SQ FT 0.32 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-202	WATER PREHEATER	3,100 SQ FT 27.9 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-203	STEAM GENERATOR	5,300 SQ FT 43.1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-204	COOLER	700 SQ FT 4.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-205	COOLER	600 SQ FT 1.1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-206	COOLER	300 SQ FT 0.9 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-207	COOLER	4,500 SQ FT 19.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-301A,B	CONDENSERS	2,000 SQ FT EA 19.3 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-302A,B	REBOILERS	1,700 SQ FT EA 20.27 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-303	PREHEATER	2,400 SQ FT 15.2 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-401	CONDENSER	6,800 SQ FT 48.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	

Table 5.7 (Continued)
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

MAJOR EQUIPMENT				
CAPACITY: 309 MILLION LB/YR (140,000 T/YR)				
CAPROLACTAM				
AT 0.90 STREAM FACTOR				
EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONCLUDED)				
E-402	COOLER	9,600 SQ FT 46.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-403A,B	CONDENSERS	2,500 SQ FT EA 17.3 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-404A,B	REBOILERS	6,300 SQ FT EA 19.9 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-405A,B	CRUDE PRODUCT COOLERS	150 SQ FT EA 2.3 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-406A,B	CONDENSERS	350 SQ FT EA 2.3 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-407A,B	REBOILERS	230 SQ FT EA 1.47 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-408A,B	PRODUCT COOLERS	580 SQ FT EA 1.9 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-409A,B	CONDENSERS	140 SQ FT EA 0.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-410	CONDENSER	330 SQ FT 3.4 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-411A,B	STIRRED KETTLES	76 SQ FT EA 0.15 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	WITH 50 HP AGITATOR
E-412A,B	CONDENSERS	55 SQ FT EA 0.2 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-501A-C	CONDENSERS	7,700 SQ FT EA 27 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-502A-C	HEATERS	1,600 SQ FT EA 27.2 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
DIRECT-FIRED HEATERS				
H-151	DOWTHERM	10.3 MMBTU/HR	C.S.	
TANKS				
T-101	CYCLOHEXANE TANK	164,800 GAL	C.S.	
T-102	SURGE TANK	510,000 GAL	C.S.	
T-103	CAUSTIC SODA TANK	73,000 GAL	C.S.	
T-104	ACETIC ACID TANK	27,200 GAL	304 SS	
T-105	SURGE TANK	93,000 GAL	316 SS	
T-106	CYCLOHEXANONE TANK	120,000 GAL	316 SS	
T-151	CYCLOHEXANE TANK	864,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-152	WASTE WATER TANK	320,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-201	NITRIC ACID	7,500 GAL	316 SS	
T-202	AMMONIUM BISULFATE	145,000 GAL	316 SS	
T-251	NITRIC ACID STORAGE	24,000 GAL	316 SS	NOT SHOWN IN FLOW DIAGRAM
T-252A,B	AMMONIA STORAGE	231,000 GAL EA	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-401	CYCLOHEXANONE OXIME TK	130,000 GAL	316 SS	
T-402	OLEUM TANK	77,000 GAL	RUBBER LINED	
T-403	AMMONIA WATER TANK	174,000 GAL	C.S.	
T-404	BENZENE TANK	196,800 GAL	304 SS	
T-405	CAPROLACTAM TANK	123,000 GAL	316 SS	
T-406	HEAVY ENDS TANK	36,000 GAL	316 SS	
T-451	OLEUM STORAGE	388,000 GAL	RUBBER LINED	NOT SHOWN IN FLOW DIAGRAM
T-452A,B	CAPROLACTAM STORAGE	388,000 GAL EA	316 SS	NOT SHOWN IN FLOW DIAGRAM

Table 5.7 (Continued)
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

MAJOR EQUIPMENT				
CAPACITY: 309 MILLION LB/YR (140,000 T/YR) CAPROLACTAM AT 0.90 STREAM FACTOR				
EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
TANKS (CONCLUDED)				
T-501	SURGE TANK	162,000 GAL	316 SS	
T-502	AMMONIUM SULFATE	33,600 GAL	316 SS	WITH HEATING COILS
PRESSURE VESSELS				
V-101	DECANTER	2,800 GAL	304 SS	
V-102A,B	CATALYST VESSELS	1,200 GAL EA	304 SS	EACH EQUIPPED WITH 10 HP TURBINE AGITATOR ONE SPARE, EACH EQUIPPED WITH 60 HP TURBINE
V-103A,B	MIXING VESSELS	8,000 GAL EA	C.S.	
AGITATOR				
V-104A-D	REFLUX DRUMS	14,600 GAL EA	C.S.	
V-105	REFLUX DRUM	1,750 GAL	304 SS	
V-106A,B	REFLUX DRUMS	240 GAL EA	C.S.	
V-107A,B	REFLUX DRUMS	1,800 GAL EA	C.S.	
V-108A,B	REFLUX DRUMS	1,700 GAL EA	C.S.	
V-109	SEPARATOR	1,700 GAL	C.S.	
V-201	CONDENSATE DRUM	1,320 GAL	316 SS	
V-202	SLURRY VESSEL	3,800 GAL	C.S.	WITH 32 HP TURBINE AGITATOR
V-203	SURGE VESSEL	3,100 GAL	316 SS CLAD	
V-301A,B	REFLUX DRUMS	2,320 GAL EA	316 SS	
V-302	DECENTER	3,000 GAL	316 SS	
V-401	DECANTER	25,000 GAL	316 SS CLAD	WITH 40 HP TURBINE AGITATOR
V-402	NEUTRALIZATION VESSEL	4,500 GAL	316 SS CLAD	
V-403	DECANTER	14,000 GAL	316 SS CLAD	
V-404A,B	REFLUX DRUM	5,100 GAL EA	304 SS CLAD	
V-405A,B	REFLUX DRUMS	100 GAL EA	316 SS	
V-406A,B	REFLUX DRUMS	90 GAL EA	316 SS	
MISCELLANEOUS EQUIPMENT				
M-101	WEIGH SCALE	50 LB DIAL	C.S.	
M-102	WEIGH SCALE	10 LB DIAL	C.S.	
M-103	VACCUM SYSTEM	45-400 MMHG	C.S.	NOT SHOWN IN FLOW DIAGRAM
M-201	STATIC MIXER	21900 LB/HR	316 SS	
M-202	EJECTOR	32400 LB/HR	316 SS	
M-203	FILTER	CARTRIDGE	316 SS	
M-204	FILTER	CARTRIDGE	316 SS	
M-205	STATIC MIXER	12000 LB/HR	316 SS	
M-206	FILTER	PRESS TYPE	316 SS	
M-401	STATIC MIXER	580000 LB/HR	316 SS	
M-402	VACCUM SYSTEM	3-200 MMHG	316 SS	NOT SHOWN IN FLOW DIAGRAM
M-501	AIR FILTER	CARTRIDGE	C.S.	
SPECIAL EQUIPMENT				
S-201	CENTRIFUGE	1.2 TONS/HR	316 SS	38 HP DRIVE WITH 13 HP DRIVE
S-401A,B	THIN FILM EVAPORATORS	100 SQFT	C.S.	
S-501A-C	CRYSTALLIZERS	250 TONS/HR	316 SS	EACH EQUIPPED WITH 20 HP DRIVE EACH EQUIPPED WITH 75 HP DRIVE
S-502A-C	THINKENERS	10050 SQFT	304 SS	
S-503A-C	CENTRIFUGES	12 TONS/HR	316 SS	EACH EQUIPPED WITH 102 HP DRIVE EACH EQUIPPED WITH 3 HP DRIVE
S-504A-C	ROTARY DRYERS	12 FT X 55 FT	316 SS	
S-505A-C	BUCKET ELEVATORS	11 TONS/HR	C.S.	EACH EQUIPPED WITH 3 HP DRIVE EACH EQUIPPED WITH 3 HP DRIVE
S-506A-C	HPPERS	6 FT X 20 FT	316 SS	
S-507A-C	SIFTERS	5 SQFT	316 SS	EACH EQUIPPED WITH 9 HP DRIVE
S-508A-C	CRUSHERS	11 TONS/HR	316 SS	
S-509A-C	BAGGING UNITS	7 BAGS/MIN	316 SS	

Table 5.7 (Concluded)
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
CAPROLACTAM
AT 0.90 STREAM FACTOR

PUMPS

SECTION	OPERATING	SPARES	OPERATING BHP
100	28	19	487
200	7	7	39
300	10	8	24
400	23	19	200
500	9	6	65

Table 5.8
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

TOTAL CAPITAL INVESTMENT			
CAPACITY: 309 MILLION LB/YR (140,000 T/YR)			
CAPROLACTAM			
AT 0.90 STREAM FACTOR			
PEP COST INDEX: 624			
	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	6,784	0.76	0.69
COLUMNS	10,504	0.83	0.60
VESSELS & TANKS	6,389	0.60	0.55
HEAT EXCHANGERS	8,955	0.87	0.78
FURNACES	228	0.79	0.79
COMPRESSORS	4,178	0.76	0.76
SPECIAL EQUIPMENT	8,894	0.63	0.63
MISCELLANEOUS EQUIPMENT	537	0.61	0.60
PUMPS	1,463	0.56	0.43

TOTAL	47,932	0.75	0.65
DIRECT INSTALLATION COSTS	64,850	0.47	0.36
INDIRECT COSTS	36,434	0.55	0.43
UNSCHEDULED EQUIPMENT, 10%	14,922	0.58	0.46

BATTERY LIMITS, INSTALLED	164,138	0.58	0.46
CONTINGENCY, 25%	41,034	0.58	0.46

BATTERY LIMITS INVESTMENT	205,172	0.58	0.46
OFF-SITES, INSTALLED			
CLARIFIED WATER	2,551	0.74	0.74
COOLING WATER	14,001	0.94	0.95
PROCESS WATER	1,366	0.62	0.62
BOILER FEED WATER	4,645	0.58	0.58
STEAM	29,967	0.92	0.91
REFRIGERATION	10,863	0.95	0.95
INERT GAS	346	0.95	0.52
TANKAGE	7,301	0.73	0.67
WAREHOUSE FACILITIES	3,619	0.70	0.70

UTILITIES & STORAGE	74,659	0.87	0.85
GENERAL SERVICE FACILITIES	55,966	0.67	0.56
WASTE TREATMENT	10,259	0.58	0.46

TOTAL	140,884	0.77	0.70
CONTINGENCY, 25%	35,221	0.77	0.70

OFF-SITES INVESTMENT	176,105	0.77	0.70

TOTAL FIXED CAPITAL	381,277	0.67	0.57

Table 5.9
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

CAPITAL INVESTMENT BY SECTION

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)

CAPROLACTAM
AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	CYCLOHEXANE OXIDATION			NITRIC OXIDE HYDROGENATION			CYCLOHEXANONE OXIMATION		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	3,189	0.72	0.65	1,860	0.76	0.66	1,156	0.88	0.81
COLUMNS	7,018	0.82	0.53	220	0.74	0.60	1,663	0.86	0.82
VESSELS & TANKS	2,515	0.56	0.53	855	0.56	0.54	97	0.41	0.42
HEAT EXCHANGERS	4,715	0.87	0.78	799	0.84	0.79	735	0.83	0.86
FURNACES	228	0.79	0.79	--	--	--	--	--	--
COMPRESSORS	4,178	0.76	0.76	--	--	--	--	--	--
SPECIAL EQUIPMENT	--	--	--	55	0.60	0.58	--	--	--
MISCELLANEOUS EQUIPMENT	62	0.62	0.62	329	0.62	0.62	--	--	--
PUMPS	694	0.67	0.55	132	0.39	0.33	109	0.28	0.24
TOTAL	22,598	0.77	0.64	4,250	0.72	0.64	3,760	0.84	0.79
DIRECT INSTALLATION COSTS	35,462	0.55	0.42	5,427	0.32	0.26	4,983	0.30	0.25
INDIRECT COSTS	18,756	0.60	0.45	3,126	0.46	0.37	2,824	0.51	0.41
UNSCHEDEDULED EQUIPMENT, 10%	7,682	0.63	0.49	1,280	0.49	0.40	1,157	0.54	0.45
BATTERY LIMITS INSTALLED	84,499	0.63	0.49	14,084	0.49	0.40	12,724	0.54	0.45
CONTINGENCY, 25%	21,125	0.63	0.49	3,521	0.49	0.40	3,181	0.54	0.45
BATTERY LIMITS INVESTMENT	105,624	0.63	0.49	17,606	0.49	0.40	15,905	0.54	0.45
OFFSITES, INSTALLED									
CLARIFIED WATER	1,475	0.74	0.74	228	0.74	0.74	109	0.74	0.74
COOLING WATER	8,286	0.94	0.95	1,000	0.94	0.95	696	0.94	0.95
PROCESS WATER	718	0.62	0.62	87	0.62	0.62	60	0.62	0.62
BOILER FEED WATER	3,270	0.58	0.58	608	0.58	0.58	130	0.58	0.58
STEAM	22,866	0.92	0.90	--	--	--	1,100	0.95	0.95
REFRIGERATION	--	--	--	4,955	0.95	0.95	--	--	--
INERT GAS	134	0.95	0.52	94	0.95	0.52	8	0.95	0.52
TANKAGE	1,190	0.65	0.65	3,178	0.82	0.69	--	--	--
WAREHOUSE FACILITIES	3,619	0.70	0.70	--	--	--	--	--	--
UTILITIES & STORAGE	41,559	0.86	0.84	10,150	0.88	0.83	2,103	0.91	0.90

Table 5.9 (Concluded)
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

CAPITAL INVESTMENT BY SECTION

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	REARRANGEMENT AND PURIFICATION			AMMONIUMSULFATE RECOVERY		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.						
REACTORS	579	0.76	0.73	--	--	--
COLUMNS	1,603	0.86	0.69	--	--	--
VESSELS & TANKS	2,212	0.67	0.58	710	0.56	0.54
HEAT EXCHANGERS	2,057	0.89	0.77	649	0.83	0.68
FURNACES	--	--	--	--	--	--
COMPRESSORS	--	--	--	--	--	--
SPECIAL EQUIPMENT	1,213	0.65	0.65	7,627	0.63	0.63
MISCELLANEOUS EQUIPMENT	126	0.57	0.56	20	0.58	0.49
PUMPS	429	0.52	0.37	98	0.39	0.30
TOTAL	8,219	0.76	0.66	9,104	0.64	0.62
DIRECT INSTALLATION COSTS	9,470	0.45	0.30	9,508	0.33	0.31
INDIRECT COSTS	5,715	0.56	0.41	6,012	0.44	0.41
UNSCHEDULED EQUIPMENT, 10%	2,340	0.59	0.44	2,462	0.48	0.45
BATTERY LIMITS INSTALLED	25,744	0.59	0.44	27,086	0.48	0.45
CONTINGENCY, 25%	6,436	0.59	0.44	6,772	0.48	0.45
BATTERY LIMITS INVESTMENT	32,181	0.59	0.44	33,858	0.48	0.45
OFFSITES, INSTALLED						
CLARIFIED WATER	510	0.74	0.74	229	0.74	0.74
COOLING WATER	2,562	0.94	0.95	1,457	0.94	0.95
PROCESS WATER	222	0.62	0.62	126	0.62	0.62
BOILER FEED WATER	350	0.58	0.58	287	0.58	0.58
STEAM	3,564	0.92	0.90	2,436	0.95	0.95
REFRIGERATION	5,908	0.95	0.95	--	--	--
INERT GAS	94	0.95	0.52	16	0.95	0.52
TANKAGE	2,933	0.65	0.65	--	--	--
WAREHOUSE FACILITIES	--	--	--	--	--	--
UTILITIES & STORAGE	16,143	0.87	0.86	4,551	0.91	0.90

Table 5.10
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
ACETIC ACID	31 ¢/LB	0.00122 LB	0.04
AMMONIA	8.75 ¢/LB	0.60351 LB	5.28
CYCLOHEXANE	15.62 ¢/LB	1.02669 LB	16.04
COBALT NAPHTHENATE	3.71 \$/LB	0.00008 LB	0.03
COBALTOUS SULFATE	2.81 \$/LB	0.00001 LB	NEGL
HYDROGEN	0.388 ¢/FT^3	6.91 FT^3	2.68
BENZENE	9.5 ¢/LB	0.008207 LB	0.08
OLEUM (32%)	4.01 ¢/LB	1.17745 LB	4.72
OXYGEN	2.017 ¢/LB	0.39465 LB	0.80
SODIUM HYDROXIDE	11 ¢/LB	0.12552 LB	1.38
SULFURIC ACID	2.23 ¢/LB	0.00008 LB	NEGL
GROSS RAW MATERIALS			31.05
BY-PRODUCTS			
AMMONIUM SULFATE	1.9 ¢/LB	-1.694 LB	-3.22
NITRIC ACID (DILUTE)	4.9 ¢/LB	-0.04363 LB	-0.21
FUEL	2.21 \$/MMBTU	-0.001 MMBTU	-0.22
TOTAL BY-PRODUCTS			-3.65
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	121 GAL	1,010 LITERS
PROCESS WATER	1.101 \$/MGAL	0.564 GAL	4.71 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	8.52 LB	8.52 KG
STEAM, 600 PSIG	5.72 \$/MLB	11.5 LB	11.5 KG
STEAM, 10 PSIG	2.8 \$/MLB	-1.18 LB	-1.18 KG
STEAM, 45 PSIG	3 \$/MLB	-2.02 LB	-2.02 KG
ELECTRICITY	4 ¢/KWH	0.148 KWH	0.327 KWH
NATURAL GAS	3.24 \$/MMBTU	351 BTU	195 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	1.12 SCF	70.2 LITERS
REFRIGERATION, 40°F	4.99 ¢/TON-HR	0.146 TON-HR	1.13 KWH
TOTAL UTILITIES			11.91

Table 5.10 (Concluded)
CAPROLACTAM FROM CYCLOHEXANE BY THE NITRIC OXIDE REDUCTIVE PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	154	309#	617
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	148.7	205.2	307.3
OFFSITES	108.6	176.1	300.9
TOTAL FIXED CAPITAL (TFC)	257.4	381.3	608.2
SCALING EXPONENTS	0.57	0.67	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	31.05	31.05	31.05
BY-PRODUCTS	-3.65	-3.65	-3.65
UTILITIES	11.91	11.91	11.91
VARIABLE COSTS	39.31	39.31	39.31
OPERATING LABOR, 12/SHIFT, \$33.58/HOUR	2.29	1.14	0.57
MAINTENANCE LABOR, 3%/YR OF BLI	2.89	1.99	1.49
CONTROL LAB LABOR, 20% OF OPER LABOR	0.46	0.23	0.11
LABOR COSTS	5.64	3.36	2.17
MAINTENANCE MATERIALS, 3%/YR OF BLI	2.89	1.99	1.49
OPERATING SUPPLIES, 10% OF OPER LABOR	0.23	0.11	0.06
TOTAL DIRECT COSTS	48.07	44.77	43.03
PLANT OVERHEAD, 80% OF LABOR COSTS	4.51	2.69	1.74
TAXES AND INSURANCE, 2%/YR OF TFC	3.34	2.47	1.97
PLANT CASH COSTS	55.92	49.93	46.74
DEPRECIATION, 10%/YR OF TFC	16.68	12.35	9.85
PLANT GATE COSTS	72.60	62.28	56.59
G&A, SALES, RESEARCH	9.00	9.00	9.00
NET PRODUCTION COST	81.60	71.28	65.59
ROI BEFORE TAXES, 25%/YR OF TFC	41.70	30.88	24.63
PRODUCT VALUE	123.30	102.16	90.22

* OF CAPROLACTAM

BASE CASE

CAPM FROM CYCLOHEXANE BY HPO PROCESS

Process Description

This process combines part of the operations described in the previous two processes. The production of cyclohexanone is carried out the same way as that described in the nitric oxide process, and the oxidation of cyclohexanone is operated similarly as that described in the HPO process. The utilities summary and a major equipment list are given in Table 5.11 and 5.12, respectively. The description of the process is thus omitted.

Economics

Capital investment summary for this process is given in Table 5.13, and those for operation sections are listed in Table 5.14. At a capacity of 309 million lb/yr (140,000 t/yr), the process requires \$266.3 million for the battery limits and \$466.8 million for total fixed capital.

The production costs are summarized in Table 5.15. With a unit price of cyclohexane at 15.62 ¢/lb, the cash cost and the plant gate cost for CAPM are estimated at 58.5 ¢/lb and 73.6 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 120.5 ¢/lb.

Table 5.11
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

UTILITIES SUMMARY

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

UNITS	BATTERY LIMITS	SECTION	SECTION	SECTION	SECTION	SECTION	SECTION	
	TOTAL	100	200	300	400	500	600	
<hr/>								
AVERAGE CONSUMPTIONS								
COOLING WATER	GPM	95,400	51,200	21,000	8,200	--	5,800	9,200
PROCESS WATER	GPM	332	83	6	220	23	--	--
ELECTRICITY	KW	13,591	4,400	7,600	240	300	390	660
NATURAL GAS	MM BTU/HR	14	14	0	--	--	--	--
INERT GAS, LOW P	M SCF/HR	25	25	--	--	--	--	--
STEAM, 50 PSIG	M LB/HR	103	--	43	--	--	60	--
STEAM, 150 PSIG	M LB/HR	546	160	180	--	--	86	120
STEAM, 300 PSIG	M LB/HR	2	--	2	--	--	--	--
STEAM, 600 PSIG	M LB/HR	390	390	--	--	--	--	--
STEAM, 50 PSIG	M LB/HR	-79	-79	--	--	--	--	--
STEAM, 300 PSIG	M LB/HR	-43	--	-43	--	--	--	--
REFRIGERATION, 40°F	TONS	6,900	--	6,900	--	--	--	--

Table 5.12
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-203	METHANIZER	3 FT DIA 19 FT T-T	SHELL: C.S. PACKING: SILICA GEL	12 FT OF PACKING 12 FT OF 1/8 IN NICKEL-BASED
R-105	DEHYDROGENATION REACTR	8,220 SQ FT 10 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	785 TUBES OF 2 IN DIAMETER AND 20 FT LONG
R-101	OXIDATION REACTORS	24,000 GAL	CLADDING: 316 SS AGITATOR: 304 SS	JACKETED AND WITH 200 HP TURBINE AGITATOR
R-102	OXIDATION REACTORS	24,000 GAL	CLADDING: 316 SS AGITATOR: 304 SS	JACKETED AND WITH 200 HP TURBINE AGITATOR
R-103	OXIDATION REACTORS	24,000 GAL	CLADDING: 316 SS AGITATOR: 304 SS	JACKETED AND WITH 200 HP TURBINE AGITATOR
R-104	OXIDATION REACTORS	24,000 GAL	CLADDING: 316 SS AGITATOR: 304 SS	JACKETED AND WITH 200 HP TURBINE AGITATOR
R-201	AMMONIA OXIDIZER	16,000 GAL	CLADDING: 316 SS	
R-202A,B	NITRATE HYDROGENATORS	16,000 GAL	CLADDING: 316 SS AGITATOR: 304 SS	EACH EQUIPPED WITH 160 HP TURBINE AGITATOR AND 5800 SQFT HEAT EXCHANGER
R-204A,B	MAIN OXIMATORS	32,500 GAL	CLADDING: 316 SS AGITATOR: 304 SS	EACH EQUIPPED WITH 435 HP TURBINE AGITATOR
R-205	POST OXIMATOR	20,000 GAL	CLADDING: 316 SS AGITATOR: 304 SS	WITH 260 HP TURBINE AGITATOR
R-301A,B	REARRANGEMENT REACTORS	36,200 GAL	SHELL: C.S.	EACH WITH SPECIAL MIXING DEVICE AND EXTERNAL CIRCULATN LOOPS
R-501	HYDROGENATOR	10,500 GAL	CLADDING: 316 SS AGITATOR: 304 SS	
COLUMNS				
C-101	SCRUBBER	2.5 FT DIA 64 FT	CLADDING: 304 SS PACKING: 316 SS	50 FT OF 1 INCH RING PACKING
C-102	SRTIPPER	8 FT DIA 64 FT	CLADDING: 304 SS TRAYS: 316 SS	26 VALVE TRAYS, 24 INCH SPACING
C-103	DECOMPOSITION COLUMN	13 FT DIA 34 FT	CLADDING: 316 SS TRAYS: 316 SS	8 SIEVE TRAYS, 36 INCH SPACING WITH 8 ROTARY DICS AND 120 HP RIVE
C-104A-D	CYCLOHEXANE COLUMNS	16 FT DIA 85 FT	CLADDING: 304 SS TRAYS: 316 SS	25 VALVE TRAYS, 36 INCH SPACING
C-105	SAPONIFICATION COLUMN	3 FT DIA 40 FT	CLADDING: 316 SS TRAYS: 316 SS	15 VALVE TRAYS, 24 INCH SPACING WITH 15 ROTARY DICS, 20 HP DRIVE
C-106	WASHING COLUMN	3.5 FT DIA 28 FT	CLADDING: 316 SS PACKING: 316 SS	24 FT OF 1 INCH RING PACKING
C-107	DEHYDRATION COLUMN	8.5 FT DIA 34 FT	CLADDING: 316 SS TRAYS: 316 SS	12 VALVE TRAYS, 24 INCH SPACING
C-108A,B	LIGHT ENDS COLUMNS	9 FT DIA 200 FT	CLADDING: 304 SS TRAYS: 316 SS	95 SIEVE TRAYS, 24 INCH SPACING
C-109A,B	CYCLOHEXANONE COLUMNS	14 FT DIA 130 FT	CLADDING: 304 SS TRAYS: 316 SS	60 SIEVE TRAYS, 24 INCH SPACING
C-110A,B	CYCLOHEXANOL COLUMNS	9 FT DIA 68 FT	CLADDING: 304 SS TRAYS: 316 SS	29 SIEVE TRAYS, 24 INCH SPACING
C-201	NITROGEN OXIDE ABSORB	5.5 FT DIA 45 FT	CLADDING: 316 SS PACKING: 316 SS	32 FT OF 1 INCH RING PACKING
C-202	DECOMPOSER	4 FT DIA 30 FT	CLADDING: 316 SS PACKING: 316 SS	20 FT OF 1 INCH RING PACKING
C-203	EXTRACTOR	11 FT DIA 18 FT	CLADDING: 316 SS TRAYS: 316 SS	8 SIEVE TRAYS, 24 INCH SPACING 8 ROTARY DISCS AND 88 HP DRIVE

Table 5.12 (Continued)
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
COLUMNS (CONCLUDED)				
C-204	STRIPPER	10 FT DIA 55 FT	CLADDING: 316 SS TRAYS: 316 SS	15 SIEVE TRAYS, 36 INCH SPACING
C-205	TOLUENE COLUMN	14 FT DIA 34 FT	CLADDING: 316 SS TRAYS: 316 SS	8 SIEVE TRAYS, 36 INCH SPACING
C-206	OXIME RECTIFIER	14 FT DIA 50 FT	CLADDING: 316 SS TRAYS: 316 SS	20 SIEVE TRAYS, 24 INCH SPACING
C-401	SULFATE REMOVAL COLUMN	6.3 FT DIA 46 FT	CLADDING: 316 SS TRAYS: 316 SS	17 VALVE TRAYS, 24 INCH SPACING WITH 17 ROTARY DISCS AND 88 HP DRIVE
C-402	BENZENE EXTRACTOR	5.5 FT DIA 46 FT	CLADDING: 316 SS TRAYS: 316 SS	17 VALVE TRAYS, 24 INCH SPACING WITH 17 ROTARY DISCS AND 65 HP DRIVE
C-403	WATER WASH COLUMN	5.5 FT DIA 46 FT	CLADDING: 316 SS PACKING: PORCELAIN	36 FT OF 1 INCH RING PACKING
C-404	SECONDARY BENZENE COLN	4 FT DIA 46 FT	SHELL: 316 SS PACKING: PORCELAIN	36 FT OF 1 INCH RING PACKING
C-405	WATER EXTRACTION COLN	6.4 FT DIA 46 FT	CLADDING: 316 SS TRAYS: 316 SS	17 VALVE TRAYS, 24 INCH SPACING WITH 17 ROTARY DISCS, 90 HP DRIVE
C-501A,B	ION EXCHANGERS	6.8 FT DIA 20 FT	CLADDING: 316 SS PACKING: ALUMINA	14 FT OF PACKING
C-502	LIGHT ENDS COLUMN	2 FT DIA 40 FT	SHELL: 316 SS PACKING: 316 SS	30 FT OF 1 INCH RING PACKING
C-503A-C	PRODUCT COLUMNS	10 FT DIA 20 FT	CLADDING: 316 SS PACKING: 316 SS	10 FT OF 1 INCH RING PACKING
C-504	HEAVY ENDS COLUMN	7.7 FT DIA 20 FT	CLADDING: 316 SS PACKING: 316 SS	10 FT OF 1 INCH RING PACKING
COMPRESSORS				
K-101	AIR COMPRESSOR	3,860 BHP	C.S.	
K-201	COMPRESSOR	6,700 BHP	C.S.	WITH A 2370 SQFT INTERCOOLER
K-501	COMPRESSOR	14 BHP	316 SS	
HEAT EXCHANGERS				
E-101	CONDENSER	2,000 SQ FT 5.2 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-102	REACTANT PREHEATER	7,400 SQ FT 55 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-103	COOLER	4,000 SQ FT 53.1 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-104A-D	CONDENSERS	12,100 SQ FT 79.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-105A-D	REBOILERS	6,100 SQ FT 83 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-106	COOLER	80 SQ FT 1.11 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-107	COOLER	350 SQ FT 3.32 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-108	CONDENSER	1,320 SQ FT 5.1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-109	REBOILER	5,300 SQ FT 10.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-110A,B	CONDENSERS	900 SQ FT 10.8 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-111A,B	REBOILERS	1,570 SQ FT 10.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	

Table 5.12 (Continued)
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONTINUED)				
E-112A,B	CONDENSERS	2,330 SQ FT 13.6 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-113A,B	REBOILERS	1,000 SQ FT 13.9 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-114A,B	CONDENSERS	750 SQ FT 5.75 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-115A,B	REBOILERS	900 SQ FT 6.04 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-116	VAPORIZER	1,000 SQ FT 8.2 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-117	CONDENSER	1,700 SQ FT 11.7 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-201	AMMONIA EVAPORATOR	260 SQ FT 4.6 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-202	AMMONIA SUPERHEATER	200 SQ FT 1.3 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-203	AIR PREHEATER	1,660 SQ FT 3.4 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-204	HEAT EXCHANGER	1,800 SQ FT 40.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-205	HEAT EXCHANGER	2,250 SQ FT 8.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-206	COOLER	2,570 SQ FT 16.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-207	HEATER	130 SQ FT 0.33 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-208	COOLER	100 SQ FT 0.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-209	CONDENSER	2,630 SQ FT 85 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-210	REBOILER	3,560 SQ FT 134.3 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-211	COOLER	6,460 SQ FT 50 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-212	CONDENSER	11,030 SQ FT 38.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-213	REBOILER	5,780 SQ FT 39.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-214	CONDENSER	1,640 SQ FT 12.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-215	REBOILER	2,620 SQ FT 14.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-301A,B	COOLERS	2,560 SQ FT 17.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-302	COOLER	8,070 SQ FT 46.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-501	CONDENSER	3,940 SQ FT 35.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-502A,B	CONDENSERS	130 SQ FT 4.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-503	CONDENSER	25 SQ FT 0.2 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-504A-C	CONDENSERS	420 SQ FT 3.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-505	CONDENSER	220 SQ FT 2 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	

Table 5.12 (Continued)
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONCLUDED)				
E-601A-C	CONDENSERS	8,680 SQ FT 30.8 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
DIRECT-FIRED HEATERS				
H-101	DOWTHERM FURNACE	10.3 MMBTU/HR	CHROME-MOLY	NOT SHOWN IN FLOW DIAGRAM
H-201	DOWTHERM FURNACE	0.33 MMBTU/HR	CHROME-MOLY	NOT SHOWN IN FLOW DIAGRAM
TANKS				
T-101	CYCLOHEXANE TANK	164,800 GAL	C.S.	
T-102	SUREG TANK	10,000 GAL	C.S.	
T-103	CAUSTIC SODA TANK	73,000 GAL	C.S.	
T-104	ACETIC ACID TANK	27,200 GAL	304 SS	
T-105	SUREGE TANK	93,000 GAL	316 SS	
T-106	CYCLOHEXANONE TANK	120,000 GAL	316 SS	
T-151	CYCLOHEXANE STORAGE	864,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-152	WASTE WATER TANK	320,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-201	HYDROXYL AMMONIUM TK	550,000 GAL	316 SS	
T-202	TOLUENE TANK	243,000 GAL	C.S.	
T-251A,B	AMMONIA STORAGE	52,000 GAL	NI LINED	NOT SHOWN IN FLOW DIAGRAM
T-252	WASTE WATER TANK	353,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-301	OLEUM TANK	85,600 GAL	RUBBER LINED	
T-302	AMMONIA WATER	176,000 GAL	C.S.	
T-303	CRUDE CAPM TANK	68,700 GAL	316 SS	
T-351	OLEUM STORAGE	428,000 GAL	RUBBER LINED	NOT SHOWN IN FLOW DIAGRAM
T-401	LACTAM-BENZENE TANK	297,400 GAL	316 SS	
T-501	CAPM SURGE TANK	183,800 GAL	316 SS	
T-502	CAUSTIC SODA TANK	50 GAL	316 SS	
T-503	CRUDE CAPM TANK	71,600 GAL	316 SS	WITH HEATING COILS
T-504	PURIFIED CAPM TANK	125,000 GAL	316 SS	WITH HEATING COILS
T-551A,B	CAPM STORAGE	320,000 GAL	316 SS	NOT SHOWN IN FLOW DIAGRAM
T-601	AMMONIUM SULFATE TANK	186,000 GAL	C.S.	WITH HEATING COILS
T-602	MOTHER LIQUOR TANK	37,700 GAL	304 SS	WITH HEATING COILS
PRESSURE VESSELS				
V-101	DECANTER	2,800 GAL	304 SS CLAD	
V-102A,B	CATALYST VESSELS	1,200 GAL	316 SS	EACH EQUIPPED WITH 10 HP TURBINE AGITATOR
V-103A,B	MIXING VESSELS	8,000 GAL	C.S.	EACH EQUIPPED WITH 60 HP TURBINE AGITATOR
V-104A-D	REFLUX DRUMS	14,600 GAL	C.S.	
V-105	REFLUX DRUM	750 GAL	304 SS	
V-106A,B	REFLUX DRUMS	2,400 GAL	C.S.	
V-107A,B	REFLUX DRUMS	1,800 GAL	C.S.	
V-108A,B	REFLUX DRUMS	700 GAL	C.S.	
V-109	SEPARATION DRUM	1,700 GAL	C.S.	
V-201	COPRECIPITATION VESSEL	29,600 GAL	316 SS CLAD	WITH 250 HP TURBINE AGITATOR
V-202A,B	REAGENT VESSELS	1,850 GAL	316 SS	WITH 18 HP TRUBINE AGITATOR
V-203	HIGH PRESSURE SEPARATR	20,500 GAL	316 SS CLAD	
V-204	DECANTER	32,500 GAL	316 SS CLAD	
V-205	REFLUX DRUM	3,770 GAL	C.S.	
V-206	DECANTER	17,540 GAL	316 SS CLAD	
V-207	REFLUX DRUM	11,060 GAL	C.S.	
V-208	REFLUX DRUM	3,100 GAL	C.S.	

Table 5.12 (Continued)
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
PRESSURE VESSELS (CONCLUDED)				
V-301	OXIME SURGE VESSEL	54,950 GAL	316 SS CLAD	
V-302	NEUTRALIZATION VESSEL	4,780 GAL	316 SS CLAD	WITH 48 HP TURBINE AGITATOR
V-303	DECANTER	13,080 GAL	316 SS CLAD	
V-401	DECANTER	5,900 GAL	316 SS CLAD	
V-402	PH ADJUSTMENT VESSEL	5,170 GAL	316 SS CLAD	WITH 45 HP TURBINE AGITATOR
V-403	DECANTER	3,940 GAL	316 SS CLAD	
V-501A,B	CATALYST VESSELS	300 GAL	316 SS	WITH 4 HP TURBINE AGITATOR
V-502A,B	RECEIVERS	190 GAL	316 SS	
V-503	REFLUX DRUM	45 GAL	316 SS	
V-504A-C	REFLUX DRUMS	650 GAL	316 SS	
V-505	REFLUX DRUM	380 GAL	316 SS	
V-601A-C	CONDENSATE RECEIVERS	1,350 GAL	C.S.	
MISCELLANEOUS EQUIPMENT				
M-101	WEIGH SCALE'	50 LB DIAL	CARBON STEEL	
M-102	WEIGH SCALE'	10 LB DIAL	CARBON STEEL	
M-103	VACUUM SYSTEM	45-400 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-201	AIR FILTER	136200 LB/HR	316 SS	
M-202	WEIGH SCALE	100 LB DIAL	CARBON STEEL	
M-203	FILTER	CARTRIDGE	316 SS	
M-204	FILTER	CARTRIDGE	316 SS	
M-205	VACUUM SYSTEM	60-150 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-301A,B	STATIC MIXERS	1450 GPM	316 SS	
M-401	STATIC MIXER	440 GPM	316 SS	
M-402	VACUUM SYSTEM	100 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-501	WEIGH SCALE	100 LB DIAL	CARBON STEEL	
M-502	FLITER	CARTRIDGE	316 SS	
M-503	VACUUM SYSTEM	5-10 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-601	VACUUM SYSTEM	150 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
SPECIAL EQUIPMENT				
S-501A-C	EVAPORATORS	1800 SQFT	316 SS	TRIPLE EFFECT EVAPORATORS
S-504A,B	EVAPORATORS	445 SQFT	316 SS	THIN FILM EVAPORATORS EACH WITH 50 HP DRIVE
S-505	EVAPORATOR	101 SQFT	316 SS	THIN FILM EVAPORATOR WITH 20 HP DRIVE
S-506A-C	EVAPORATORS	440 SQFT	316 SS	THIN FILM EVAPORATORS EACH WITH 50 HP DRIVE
S-507	EVAPORATOR	268 SQFT	316 SS	THIN FILM EVAPORATOR WITH 30 HP DRIVE
S-601A-C	CRYSTALLIZERS	260 TONS/DAY	316 SS	EACH EQUIPPED WITH 21 HP DRIVE
S-602A-C	THICKENERS	260 TONS/DAY	316 SS	EACH EQUIPPED WITH 80 PH DRIVE
S-603A-C	CENTRIFUGES	13 TONS/HR	316 SS	EACH EQUIPPED WITH 102 HP DRIVE
S-604A-C	ROTARY DRYERS	12 FT X 55 FT	CARBON STEEL	
TANKS				
S-605A-C	BUCKET ELEVATORS	12 TONS/HR	316 SS	EACH EQUIPPED WITH 3 HP DRIVE
S-606A-C	HOPPERS	6 FT X 20 FT	316 SS	
S-607A-C	SIFTERS	6 SQFT	316 SS	SINGLE DECK
S-608A-C	CRUSHERS	12 TONS/HR	316 SS	EACH EQUIPPED WITH 9 HP DRIVE
S-609A-C	BAGGING UNITS	7 BAGS/MIN	316 SS	

Table 5.12 (Concluded)
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

MAJOR EQUIPMENT

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
CAPROLACTAM
AT 0.90 STREAM FACTOR

PUMPS

SECTION	OPERATING	SPARES	OPERATING BHP
100	28	19	487
200	21	19	434
300	7	7	236
400	6	6	78
500	12	10	82
600	12	8	118

Table 5.13
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

TOTAL CAPITAL INVESTMENT			
CAPACITY: 309 MILLION LB/YR (140,000 T/YR)			
CAPROLACTAM			
AT 0.90 STREAM FACTOR			
PEP COST INDEX: 624			
	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	7,068	0.73	0.67
COLUMNS	11,588	0.83	0.62
VESSELS & TANKS	7,957	0.64	0.59
HEAT EXCHANGERS	9,375	0.88	0.79
FURNACES	270	0.79	0.79
COMPRESSORS	6,759	0.86	0.76
SPECIAL EQUIPMENT	15,503	0.69	0.67
MISCELLANEOUS EQUIPMENT	447	0.60	0.59
PUMPS	2,332	0.57	0.46

TOTAL	61,300	0.76	0.67
DIRECT INSTALLATION COSTS	86,747	0.46	0.37
INDIRECT COSTS	45,609	0.52	0.41
UNSCHEDULED EQUIPMENT, 10%	19,366	0.58	0.47

BATTERY LIMITS, INSTALLED	213,021	0.58	0.47
CONTINGENCY, 25%	53,255	0.58	0.47

BATTERY LIMITS INVESTMENT	266,277	0.58	0.47
OFF-SITES, INSTALLED			
CLARIFIED WATER	2,751	0.74	0.74
COOLING WATER	16,655	0.94	0.95
PROCESS WATER	1,496	0.62	0.62
BOILER FEED WATER	4,032	0.58	0.58
STEAM	31,218	0.95	0.91
REFRIGERATION	12,907	0.95	0.90
INERT GAS	258	0.52	0.52
TANKAGE	5,124	0.66	0.65
WAREHOUSE FACILITIES	3,744	0.60	0.60

UTILITIES & STORAGE	78,185	0.88	0.85
GENERAL SERVICE FACILITIES	68,892	0.65	0.55
WASTE TREATMENT	13,314	0.58	0.47

TOTAL	160,391	0.76	0.68
CONTINGENCY, 25%	40,098	0.76	0.68

OFF-SITES INVESTMENT	200,489	0.76	0.68
TOTAL FIXED CAPITAL	466,766	0.66	0.56

Table 5.14
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

CAPITAL INVESTMENT BY SECTION

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)
 CAPROLACTAM
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	CYCLOHEXANE OXIDATION			CYCLOHEXANONE OXIMATION			OXIME REARRANGEMENT		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	3,189	0.68	0.63	3,267	0.79	0.71	377	0.70	0.70
COLUMNS	7,179	0.83	0.56	1,963	0.85	0.72	--	--	--
VESSELS & TANKS	2,254	0.58	0.56	2,035	0.67	0.64	954	0.71	0.62
HEAT EXCHANGERS	4,867	0.88	0.78	2,806	0.89	0.83	841	0.90	0.83
FURNACES	248	0.79	0.79	22	0.79	0.74	--	--	--
COMPRESSORS	2,714	0.76	0.76	3,952	0.92	0.76	--	--	--
SPECIAL EQUIPMENT	--	--	--	--	--	--	--	--	--
MISCELLANEOUS EQUIPMENT	62	0.60	0.60	140	0.61	0.61	22	0.58	0.58
PUMPS	717	0.56	0.48	678	0.57	0.48	378	0.73	0.57
TOTAL	21,230	0.78	0.64	14,863	0.83	0.73	2,572	0.77	0.69
DIRECT INSTALLATION COSTS	29,704	0.45	0.36	26,544	0.57	0.46	3,191	0.45	0.35
INDIRECT COSTS	15,691	0.52	0.40	12,756	0.60	0.48	1,775	0.53	0.42
UNSCHEDULED EQUIPMENT, 10%	6,663	0.58	0.45	5,416	0.65	0.53	754	0.59	0.47
BATTERY LIMITS INSTALLED	73,288	0.58	0.45	59,580	0.65	0.53	8,292	0.59	0.47
CONTINGENCY, 25%	18,322	0.58	0.45	14,895	0.65	0.53	2,073	0.59	0.47
BATTERY LIMITS INVESTMENT	91,610	0.58	0.45	74,475	0.65	0.53	10,365	0.59	0.47
OFFSITES, INSTALLED									
CLARIFIED WATER	1,316	0.74	0.74	722	0.74	0.74	305	0.74	0.74
COOLING WATER	8,170	0.94	0.95	4,782	0.94	0.95	1,309	0.94	0.95
PROCESS WATER	680	0.62	0.62	398	0.62	0.62	109	0.62	0.62
BOILER FEED WATER	2,398	0.58	0.58	750	0.58	0.58	--	--	--
STEAM	22,112	0.95	0.94	3,780	0.95	0.86	--	--	--
REFRIGERATION	--	--	--	12,907	0.95	0.90	--	--	--
INERT GAS	258	0.52	0.52	--	--	--	--	--	--
TANKAGE	--	--	--	2,429	0.67	0.65	623	0.65	0.65
WAREHOUSE FACILITIES	--	--	--	--	--	--	--	--	--
TOTAL	34,935	0.91	0.89	25,769	0.90	0.86	2,345	0.83	0.82

Table 5.14 (Concluded)

**CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS**

CAPITAL INVESTMENT BY SECTION

CAPACITY: 309 MILLION LB/YR (140,000 T/YR)

CAPROLACTAM
AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	CAPROLACTAM EXTRACTION			CAPROLACTAM PURIFICATION			AMMONIUMSULFATE RECOVERY		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	--	--	--	235	0.68	0.64	--	--	--
COLUMNS	816	0.61	0.49	1,629	0.87	0.84	--	--	--
VESSELS & TANKS	964	0.64	0.63	1,368	0.62	0.59	382	0.77	0.43
HEAT EXCHANGERS	--	--	--	433	0.84	0.80	428	0.95	0.63
FURNACES	--	--	--	--	--	--	--	--	--
COMPRESSORS	--	--	--	92	0.76	0.76	--	--	--
SPECIAL EQUIPMENT	--	--	--	7,729	0.75	0.72	7,774	0.63	0.63
MISCELLANEOUS EQUIPMENT	82	0.55	0.54	121	0.62	0.62	20	0.58	0.49
PUMPS	143	0.53	0.44	267	0.41	0.32	150	0.43	0.33
TOTAL	2,005	0.62	0.56	11,875	0.75	0.71	8,754	0.65	0.61
DIRECT INSTALLATION COSTS	3,444	0.31	0.30	13,576	0.34	0.29	10,289	0.39	0.33
INDIRECT COSTS	1,678	0.36	0.31	7,841	0.47	0.40	5,867	0.44	0.38
UNSCHEDULED EQUIPMENT, 10%	713	0.42	0.37	3,329	0.53	0.45	2,491	0.50	0.43
BATTERY LIMITS INSTALLED	7,840	0.42	0.37	36,621	0.53	0.45	27,400	0.50	0.43
CONTINGENCY, 25%	1,960	0.42	0.37	9,155	0.53	0.45	6,850	0.50	0.43
BATTERY LIMITS INVESTMENT	9,799	0.42	0.37	45,776	0.53	0.45	34,250	0.50	0.43
OFFSITES, INSTALLED									
CLARIFIED WATER	13	0.74	0.74	162	0.74	0.74	232	0.74	0.74
COOLING WATER	--	--	--	926	0.94	0.95	1,468	0.94	0.95
PROCESS WATER	--	--	--	77	0.62	0.62	122	0.62	0.62
BOILER FEED WATER	--	--	--	485	0.58	0.58	398	0.58	0.58
STEAM	--	--	--	2,518	0.95	0.86	2,807	0.95	0.86
REFRIGERATION	--	--	--	--	--	--	--	--	--
INERT GAS	--	--	--	--	--	--	--	--	--
TANKAGE	--	--	--	2,073	0.65	0.65	--	--	--
WAREHOUSE FACILITIES	--	--	--	--	--	--	3,744	0.60	0.60
UTILITIES & STORAGE	13	0.74	0.74	6,241	0.82	0.77	8,772	0.78	0.74

Table 5.15
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
AMMONIA	8.75 ¢/LB	0.65815 LB	5.76
HYDROGEN	0.388 ¢/FT ³	11.19 FT ³	4.34
OLEUM (7%)	4.01 ¢/LB	1.29795 LB	5.20
CYCLOHEXANE	15.62 ¢/LB	1.02669 LB	16.04
CATALYSTS AND OTHER CHEM	1.88 ¢/LB	1 LB	1.88
GROSS RAW MATERIALS			33.22
BY-PRODUCTS			
AMMONIUM SULFATE	1.9 ¢/LB	-1.778 LB	-3.38
FUEL	2.21 \$/MMBTU	-0.001 MMBTU	-0.22
TOTAL BY-PRODUCTS			-3.60
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	146 GAL	1,220 LITERS
PROCESS WATER	1.101 \$/MGAL	0.509 GAL	4.25 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	13.5 LB	13.5 KG
STEAM, 600 PSIG	5.72 \$/MLB	9.96 LB	9.96 KG
ELECTRICITY	4 ¢/KWH	0.347 KWH	0.766 KWH
NATURAL GAS	3.24 \$/MMBTU	362 BTU	201 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.639 SCF	39.9 LITERS
REFRIGERATION, 40°F	4.99 ¢/TON-HR	0.176 TON-HR	1.37 KWH
TOTAL UTILITIES			15.37

Table 5.15 (Concluded)
CAPROLACTAM FROM CYCLOHEXANE BY HYDROXYLAMINE
PHOSPHATE OXIME PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	154	309#	617
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	192.3	266.3	396.8
OFFSITES	125.1	200.5	340.4
TOTAL FIXED CAPITAL (TFC)	317.4	466.8	737.1
SCALING EXPONENTS	0.56	0.66	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	33.22	33.22	33.22
BY-PRODUCTS	-3.60	-3.60	-3.60
UTILITIES	15.37	15.37	15.37
VARIABLE COSTS	44.99	44.99	44.99
OPERATING LABOR, 15/SHIFT, \$33.58/HOUR	2.86	1.43	0.72
MAINTENANCE LABOR, 3%/YR OF BLI	3.74	2.59	1.93
CONTROL LAB LABOR, 20% OF OPER LABOR	0.57	0.29	0.14
LABOR COSTS	7.17	4.31	2.79
MAINTENANCE MATERIALS, 3%/YR OF BLI	3.74	2.59	1.93
OPERATING SUPPLIES, 10% OF OPER LABOR	0.29	0.14	0.07
TOTAL DIRECT COSTS	56.19	52.03	49.78
PLANT OVERHEAD, 80% OF LABOR COSTS	5.74	3.45	2.23
TAXES AND INSURANCE, 2%/YR OF TFC	4.11	3.03	2.39
PLANT CASH COSTS	66.04	58.51	54.40
DEPRECIATION, 10%/YR OF TFC	20.57	15.13	11.94
PLANT GATE COSTS	86.61	73.64	66.34
G&A, SALES, RESEARCH	9.00	9.00	9.00
NET PRODUCTION COST	95.61	82.64	75.34
ROI BEFORE TAXES, 25%/YR OF TFC	51.42	37.82	29.86
PRODUCT VALUE	147.03	120.46	105.20

* OF CAPROLACTAM

BASE CASE

CAPM FROM BUTADIENE VIA METHYL 6-AMINOCAPROATE

Process Description

Figure 5.3 (foldout at end of report) presents the flow diagram for this process, and the utilities summary and major equipment list are given in Table 5.16 and 5.17, respectively. A brief description of the process is given below.

This process was jointly developed by DSM and DuPont and was still being tested as of 1997. PEP's design of this process is based on patents issued to DSM. The process consists of four stages. In the first stage, butadiene, carbon monoxide, and methanol are reacted in column reactors at 950 psia and 130°C (266°F) in the presence of a Pd salt and a bidentate phosphorus ligand in diphenyl ether solvent. The product consists mainly of methyl 3-pentenoate (Me3pe) and small amounts of isomers. In the second stage, Me3pe is isomerized to methyl 4-pentenoate (Me4pe) at 15 psia and 135°C (275°F) for 6 hours in a fixed-bed reactor packed with a Pd-zeolite catalyst. Unconverted Me3pe is recovered and recycled. Me4pe is then hydroformylated at 150 psia and 130°C (266°F) in column reactors using a catalyst consisting of Rh compound and tris-(m-sulfonatophenyl) phosphine. Unreacted Me4pe is recovered and recycled. Methyl 5-formylvalerate (Me5fv) is then separated from its isomers. In the third stage, Me5fv is reacted with hydrogen and anhydrous ammonia at 1470 psia and 130°C (266°F) to give methyl 6-aminocaproate in a fixed-bed reactor packed with a Ru-alumina catalyst. Unreacted ammonia and Me5fv are recovered and recycled. In the last stage, the product is sent to a multitubular reactor along with a xylene stream, where it is cyclized to caprolactam at 1470 psia and 270 °C (518°F). Methanol regenerated during cyclization is recovered and recycled to the first stage. Overall yield of caprolactam is about 86.3% based on the butadiene feed.

Economics

Capital investment summary for this process is given in Table 5.18, and those for operation sections are listed in Table 5.19. At a capacity of 300 million lb/yr (136,000 t/yr), the process requires \$232.1 million for the battery limits and \$394.7 million for total fixed capital.

The production costs are summarized in Table 5.20. With a unit price of butadiene at 13 ¢/lb, the cash cost and the plant gate cost for CAPM are estimated at 41.1 ¢/lb and 54.3 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 96.2 ¢/lb.

Table 5.16
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

UTILITIES SUMMARY						
CAPACITY: 300 MILLION LB/YR (136,000 T/YR)						
CAPM						
AT 0.90 STREAM FACTOR						
UNITS	BATTERY LIMITS TOTAL	SECTION 100	SECTION 200	SECTION 300	SECTION 400	
AVERAGE CONSUMPTIONS						
COOLING WATER	GPM	87,994	11,711	48,972	3,381	23,930
ELECTRICITY	KW	9,608	483	619	7,507	999
INERT GAS, LOW P	M SCF/HR	6	2	--	--	4
STEAM, 150 PSIG	M LB/HR	735	19	513	43	160
STEAM, 1500 PSIG	M LB/HR	225	18	200	--	7
REFRIGERATION, 20°F	TONS	1,545	108	--	875	562

Table 5.17
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 CAPM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101A-C	CARBONYLATION REACTORS	8 FT DIA 60 FT T-T	SHELL: 304 SS PACKING: ACTIVATED CARBON	29 FT OF PACKING EACH EQUIPPED WITH COOLING COILS
R-201	ISOMERIZOR	8 FT DIA 40 FT T-T	CLADDING: 304 SS PACKING: PORCELAIN	20 FT OF 1 INCH BERL PACKING WITH 20 FT OF SILICA PACKING
R-202A-C	HYDROFORMYLATORS	9 FT DIA 70 FT T-T	CLADDING: 304 SS PACKING: PORCELAIN	50 FT OF 1 INCH BERL PACKING EACH EQUIPPED WITH COOLING COILS
R-301	AMINATION REACTOR	7 FT DIA 56 FT T-T	SHELL: 304 SS PACKING: PORCELAIN	45 FT OF 1 INCH RING PACKING
R-401	CYCLIZATION	8 FT DIA 22 FT T-T	SHELL: 304 SS PACKING: SILICA GEL	12 FT OF PACKING
COLUMNS				
C-101	BD RECOVERY	6 FT DIA 60 FT	CLADDING: 304 SS TRAYS: 304 SS	33 VALVE TRAYS, 18 INCH SPACING
C-102	METHANOL RECOVERY COLM	6.5 FT DIA 73 FT	CLADDING: 304 SS TRAYS: 304 SS	42 VALVE TRAYS, 18 INCH SPACING
C-103	CATALYST RECOVERY COLU	10.5 FT DIA 64 FT	CLADDING: 304 SS TRAYS: 304 SS	27 VALVE TRAYS, 24 INCH SPACING
C-104A,B	DRYING COLUMNS	8 FT DIA 28 FT	CLADDING: 304 SS PACKING: 316 SS	18 FT OF 1 INCH RING PACKING
C-201A,B	PENTENOATES SPLITTER	16 FT DIA 190 FT	CLADDING: 304 SS TRAYS: 304 SS	89 SIEVE TRAYS, 24 INCH SPACING
C-202	CATALYST COLUMN	7 FT DIA 36 FT	CLADDING: 304 SS TRAYS: 304 SS	17 VALVE TRAYS, 18 INCH SPACING
C-203	METHYL-2-PENTENOATE SP	16 FT DIA 190 FT	CLADDING: 304 SS TRAYS: 304 SS	92 VALVE TRAYS, 24 INCH SPACING
C-204	PENTENOATE-VALERATE SP	6 FT DIA 63 FT	CLADDING: 304 SS TRAYS: 304 SS	35 VALVE TRAYS, 18 INCH SPACING
C-205	METHYL-4=ENTENOATE CL	12.5 FT DIA 142 FT	CLADDING: 304 SS TRAYS: 304 SS	88 VALVE TRAYS, 18 INCH SPACING
C-206	METHYL-5-FORMYLVALERAT	16 FT DIA 190 FT	SHELL: C.S. TRAYS: C.S.	90 VALVE TRAYS, 24 INCH SPACING
C-301	AMMONIA COULMN	6 FT DIA 36 FT	CLADDING: 304 SS TRAYS: 304 SS	17 VALVE TRAYS, 18 INCH SPACING
C-302	VALERATE RECOVERY COLN	6 FT DIA 36 FT	CLADDING: 304 SS TRAYS: 304 SS	17 VALVE TRAYS, 18 INCH SPACING
C-401	METHANOL RECOVERY COLN	12 FT DIA 62 FT	CLADDING: 304 SS TRAYS: 304 SS	26 VALVE TRAYS, 24 INCH SPACING
C-402	METHANOL-WATER SPLITTR	13 FT DIA 130 FT	CLADDING: 304 SS TRAYS: 304 SS	60 VALVE TRAYS, 24 INCH SPACING
C-403	CAPROATES RECOVERY COL	6 FT DIA 42 FT	CLADDING: 304 SS TRAYS: 304 SS	21 VALVE TRAYS, 18 INCH SPACING
C-404	CAPROLACTAM COLUMN	6.5 FT DIA 72 FT	CLADDING: 304 SS TRAYS: 304 SS	42 VALVE TRAYS, 18 INCH SPACING
COMPRESSORS				
K-101	CO COMPRESSOR	397 BHP	C.S.	
K-102	CO COMPRESSOR	53 BHP	C.S.	
K-301	HYDROGEN COMPRESSOR	465 BHP	C.S.	
K-302	H2 AND NH3 COMPRESSOR	7,796 BHP	C.S.	
K-303	H2 AND NH3 COMPRESSOR	1,654 BHP	C.S.	

Table 5.17 (Continued)
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 CAPM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS				
E-101	BUTADIENE PREHEATER	150 SQ FT 1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-102	METHANOL HEATER	350 SQ FT 2.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-103	BUTADIENE HEATER	325 SQ FT 1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-104	BUTADIENE PREHEATER	100 SQ FT 1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-105	BUTADIENE HEATER	100 SQ FT 1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-106	COOLER	1,050 SQ FT 5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-107	COOLER	200 SQ FT 2.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-108	CONDENSER	600 SQ FT 1.3 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-109	REBOILER	4,650 SQ FT 16 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-110	CONDENSER	5,775 SQ FT 16 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-111	REBOILER	1,300 SQ FT 9 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-112	CONDENSER	650 SQ FT 7.8 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-113	REBOILER	1,850 SQ FT 10 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-201A,B	REBOILERS	10,000 SQ FT 190 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-202A,B	CONDENSERS	9,900 SQ FT 275 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-203A,B	REBOILERS	1,100 SQ FT 11.3 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-204A,B	CONDENSERS	1,240 SQ FT 13.6 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-205	COOLER	3,900 SQ FT 26 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-206	CONDENSER	9,980 SQ FT 156 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-207	REBOILER	9,000 SQ FT 140 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-208	CONDENSER	625 SQ FT 4.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-209	REBOILER	1,100 SQ FT 4.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-210	HEATER	200 SQ FT 1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-211	REBOILER	1,150 SQ FT 20 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-212	CONDENSER	5,000 SQ FT 20.6 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-213	REBOILER	5,055 SQ FT 46 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-214	CONDENSER	5,600 SQ FT 43 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-215	HEATER	1,950 SQ FT 23.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	

Table 5.17 (Continued)
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 CAPM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONCLUDED)				
E-301	AMMONIA HEATER	125 SQ FT 1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-302	COOLER	130 SQ FT 1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-303	COOLER	160 SQ FT 1.2 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-304	HEATER	2,775 SQ FT 13.3 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-305	COOLER	1,235 SQ FT 7 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-306	CONDENSER	5,125 SQ FT 10.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-307	REBOILER	4,535 SQ FT 15.4 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-308	CONDENSER	6,150 SQ FT 14 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-309	REBOILER	8,035 SQ FT 8.6 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-401	COOLER	1,450 SQ FT 9 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-402	COOLER	2,125 SQ FT 9 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-403A,B	REBOILERS	9,800 SQ FT 50 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-404A,B	CONDENSERS	9,200 SQ FT 45 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-405	REBOILER	2,025 SQ FT 29 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-406	CONDENSER	6,590 SQ FT 25.15 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-407	CONDENSER	3,750 SQ FT 23 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-408	REBOILER	1,625 SQ FT 24 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-409	REBOILER	350 SQ FT 4.2 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-411	COOLER	1,240 SQ FT 10.6 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
TANKS				
T-101A-C	BUTADIENE TANKS	123,500 GAL	C.S.	
T-102	METHANOL TANK	26,000 GAL	304 SS	
T-103	SURGE TANK	10,600 GAL	304 SS	
T-301	AMMONIA TANK	19,000 GAL	C.S.	
T-351	AMMONIA STORAGE	95,000 GAL	C.S.	
T-401	CAPROLACTAM TANK	114,000 GAL	304 SS	
T-402	XYLENE TANK	2,000 GAL	304 SS	
T-451A,B	CAPROLACTAM STORAGE	320,000 GAL	304 SS	
PRESSURE VESSELS				
V-101A,B	CATALYST SOLUTION VES	5,000 GAL	304 SS CLAD	
V-102	FLASH VESSEL	8,670 GAL	316 SS CLAD	
V-103	REFLUX DRUM	1,500 GAL	316 SS CLAD	
V-104	REFLUX DRUM	1,375 GAL	316 SS CLAD	
V-105	REFLUX DRUM	11,220 GAL	316 SS CLAD	

Table 5.17 (Concluded)
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 CAPM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
PRESSURE VESSELS (CONCLUDED)				
V-201	REFLUX DRUM	28,000 GAL	316 SS CLAD	
V-202	REFLUX DRUM	9,100 GAL	316 SS CLAD	
V-203	REFLUX DRUM	34,300 GAL	316 SS CLAD	
V-204	REFLUX DRUM	2,200 GAL	316 SS CLAD	
V-205	REFLUX DRUM	10,600 GAL	316 SS CLAD	
V-206	REFLUX DRUM	23,000 GAL	316 SS CLAD	
V-207	SURGE VESSEL	11,750 GAL	316 SS CLAD	
V-301A,B	FLASH DRUMS	17,500 GAL	304 SS CLAD	
V-302	REFLUX DRUM	2,300 GAL	304 SS	
V-303	REFLUX DRUM	2,400 GAL	316 SS CLAD	
V-304	DECANTER	1,250 GAL	316 SS CLAD	
V-401	EMULSIFIER	8,400 GAL	316 SS CLAD	WITH 85 HP TURBINE AGITATOR
V-402	REFLUX DRUM	10,575 GAL	304 SS CLAD	
V-403	REFLUX DRUM	4,250 GAL	304 SS CLAD	
V-404	REFLUX DRUM	15,200 GAL	316 SS CLAD	
V-405	REFLUX DRUM	1,850 GAL	316 SS CLAD	
V-406	SURGE VESSEL	28,000 GAL	316 SS CLAD	
SPECIAL EQUIPMENT				
S-401	EVAPORATOR	600 SQFT	304 SS	THIN FILM EVAPORATOR WITH 60 HP DRIVE
PUMPS				
SECTION	OPERATING	SPARES	OPERATING BHP	
100	11	6	199	
200	15	12	830	
300	6	4	153	
400	13	10	835	

Table 5.18
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

TOTAL CAPITAL INVESTMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 CAPM
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	28,595	0.85	0.79
COLUMNS	9,475	0.93	0.73
VESSELS & TANKS	2,881	0.66	0.57
HEAT EXCHANGERS	7,974	0.89	0.76
COMPRESSORS	5,725	0.89	0.76
SPECIAL EQUIPMENT	977	0.76	0.76
PUMPS	1,453	0.71	0.60
-----	-----	-----	-----
TOTAL	57,080	0.86	0.75
DIRECT INSTALLATION COSTS	68,625	0.58	0.43
INDIRECT COSTS	43,125	0.68	0.54
UNSCHEDULED EQUIPMENT, 10%	16,883	0.70	0.56
-----	-----	-----	-----
BATTERY LIMITS, INSTALLED	185,713	0.70	0.56
CONTINGENCY, 25%	46,428	0.70	0.56
-----	-----	-----	-----
BATTERY LIMITS INVESTMENT	232,141	0.70	0.56
OFF-SITES, INSTALLED			
CLARIFIED WATER	2,360	0.74	0.74
COOLING WATER	14,560	0.94	0.95
PROCESS WATER	1,303	0.62	0.62
BOILER FEED WATER	3,961	0.59	0.59
STEAM	31,026	0.92	0.95
REFRIGERATION	4,163	0.95	0.95
INERT GAS	120	0.52	0.52
TANKAGE	2,514	0.68	0.67
-----	-----	-----	-----
UTILITIES & STORAGE	60,008	0.89	0.89
GENERAL SERVICE FACILITIES	58,430	0.74	0.62
WASTE TREATMENT	11,607	0.70	0.56
-----	-----	-----	-----
TOTAL	130,045	0.81	0.73
CONTINGENCY, 25%	32,511	0.81	0.73
-----	-----	-----	-----
OFF-SITES INVESTMENT	162,556	0.81	0.73
TOTAL FIXED CAPITAL	394,697	0.75	0.63

Table 5.19
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

CAPITAL INVESTMENT BY SECTION

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

CAPM

AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

CARBONYLATION ISOMERIZATION & HYDROFORMYLATION

	CAPACITY EXPONENT			CAPACITY EXPONENT		
	COST (\$1,000)	UP	DOWN	COST (\$1,000)	UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.						
REACTORS	9,371	0.88	0.84	13,005	0.83	0.76
COLUMNS	1,323	0.91	0.79	6,763	0.94	0.73
VESSELS & TANKS	900	0.55	0.49	568	0.71	0.60
HEAT EXCHANGERS	883	0.82	0.75	3,546	0.90	0.77
COMPRESSORS	467	0.76	0.76	--	--	--
SPECIAL EQUIPMENT	--	--	--	--	--	--
PUMPS	190	0.57	0.48	576	0.73	0.63
TOTAL	13,134	0.85	0.79	24,459	0.87	0.74
DIRECT INSTALLATION COSTS	20,064	0.36	0.32	17,634	0.65	0.38
INDIRECT COSTS	11,389	0.54	0.46	14,441	0.74	0.55
UNSCHEDULED EQUIPMENT, 10%	4,459	0.57	0.48	5,653	0.77	0.57
BATTERY LIMITS INSTALLED	49,046	0.57	0.48	62,187	0.77	0.57
CONTINGENCY, 25%	12,262	0.57	0.48	15,547	0.77	0.57
BATTERY LIMITS INVESTMENT	61,308	0.57	0.48	77,733	0.77	0.57
OFFSITES, INSTALLED						
CLARIFIED WATER	289	0.74	0.74	1,329	0.74	0.74
COOLING WATER	1,915	0.94	0.95	7,900	0.94	0.95
PROCESS WATER	171	0.62	0.62	707	0.62	0.62
BOILER FEED WATER	191	0.60	0.60	3,081	0.59	0.59
STEAM	1,562	0.91	0.95	24,362	0.92	0.95
REFRIGERATION	291	0.95	0.95	--	--	--
INERT GAS	46	0.52	0.52	--	--	--
TANKAGE	--	--	--	--	--	--
UTILITIES & STORAGE	4,466	0.89	0.90	37,379	0.89	0.90

Table 5.19 (Concluded)
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

CAPITAL INVESTMENT BY SECTION

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

CAPM

AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	REDUCTIVE AMMINATION			CYCLIZATION		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.						
REACTORS	3,157	0.84	0.78	3,063	0.84	0.78
COLUMNS	160	0.62	0.48	1,229	0.89	0.69
VESSELS & TANKS	617	0.76	0.66	797	0.65	0.57
HEAT EXCHANGERS	1,240	0.89	0.75	2,304	0.90	0.77
COMPRESSORS	5,258	0.90	0.76	--	--	--
SPECIAL EQUIPMENT	--	--	--	977	0.76	0.76
PUMPS	139	0.62	0.52	548	0.75	0.65
TOTAL	10,570	0.86	0.75	8,917	0.83	0.73
DIRECT INSTALLATION COSTS	18,310	0.76	0.65	12,617	0.55	0.38
INDIRECT COSTS	9,908	0.76	0.66	7,388	0.64	0.49
UNSCHEDULED EQUIPMENT, 10%	3,879	0.79	0.68	2,892	0.66	0.51
BATTERY LIMITS INSTALLED	42,667	0.79	0.68	31,813	0.66	0.51
CONTINGENCY, 25%	10,667	0.79	0.68	7,953	0.66	0.51
BATTERY LIMITS INVESTMENT	53,334	0.79	0.68	39,767	0.66	0.51
OFFSITES, INSTALLED						
CLARIFIED WATER	120	0.74	0.74	623	0.74	0.74
COOLING WATER	752	0.94	0.95	3,993	0.94	0.95
PROCESS WATER	67	0.62	0.62	357	0.62	0.62
BOILER FEED WATER	135	0.58	0.58	554	0.58	0.58
STEAM	984	0.95	0.95	4,118	0.94	0.95
REFRIGERATION	2,358	0.95	0.95	1,514	0.95	0.95
INERT GAS	--	--	--	74	0.52	0.52
TANKAGE	784	0.73	0.73	1,731	0.65	0.65
UTILITIES & STORAGE	5,198	0.90	0.89	12,965	0.87	0.87

Table 5.20
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
BUTADIENE	13 ¢/LB	0.560109 LB	7.28
CARBON MONOXIDE	0.24 ¢/FT^3	7.167 FT^3	1.72
HYDROGEN	0.388 ¢/FT^3	6.65692 FT^3	2.58
AMMONIA	8.75 ¢/LB	0.14998 LB	1.31
METHANOL	6.82 ¢/LB	0.049248 LB	0.34
CATALYST & MISC.	148 \$/LB	0.0001 LB	1.48
GROSS RAW MATERIALS			14.71
UTILITIES			
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
COOLING WATER	7.45 ¢/MGAL	139 GAL	1,160 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	19.3 LB	19.3 KG
STEAM, 1500 PSIG	6.16 \$/MLB	5.91 LB	5.91 KG
ELECTRICITY	4 ¢/KWH	0.252 KWH	0.557 KWH
INERT GAS, LOW P	0.51 \$/MSCF	0.15 SCF	9.35 LITERS
REFRIGERATION, 20°F	5.11 ¢/TON-HR	0.0406 TON-HR	0.315 KWH
TOTAL UTILITIES			14.61

Table 5.20 (Concluded)
CAPROLACTAM FROM BUTADIENE VIA 6-AMINOCAPROATE

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	150	300#	600
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	157.5	232.1	378.4
OFFSITES	97.7	162.6	284.6
TOTAL FIXED CAPITAL (TFC)	255.2	394.7	663.0
SCALING EXPONENTS	0.63	0.75	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	14.71	14.71	14.71
UTILITIES	14.61	14.61	14.61
VARIABLE COSTS	29.32	29.32	29.32
OPERATING LABOR, 12/SHIFT, \$33.58/HOUR	2.35	1.18	0.59
MAINTENANCE LABOR, 3%/YR OF BLI	3.15	2.32	1.89
CONTROL LAB LABOR, 20% OF OPER LABOR	0.47	0.24	0.12
LABOR COSTS	5.97	3.74	2.60
MAINTENANCE MATERIALS, 3%/YR OF BLI	3.15	2.32	1.89
OPERATING SUPPLIES, 10% OF OPER LABOR	0.23	0.12	0.06
TOTAL DIRECT COSTS	38.67	35.50	33.87
PLANT OVERHEAD, 80% OF LABOR COSTS	4.78	2.99	2.08
TAXES AND INSURANCE, 2%/YR OF TFC	3.40	2.63	2.21
PLANT CASH COSTS	46.85	41.12	38.16
DEPRECIATION, 10%/YR OF TFC	17.01	13.16	11.05
PLANT GATE COSTS	63.86	54.28	49.21
G&A, SALES, RESEARCH	9.00	9.00	9.00
NET PRODUCTION COST	72.86	63.28	58.21
ROI BEFORE TAXES, 25%/YR OF TFC	42.54	32.89	27.62
PRODUCT VALUE	115.40	96.17	85.83

* OF CAPM

BASE CASE

HMDA AND CAPM FROM ADIPONITRILE BY PARTIAL HYDROGENATION

Process Description

Figure 5.4 (foldout at end of report) presents the flow diagram for this process, and the utilities summary and major equipment list are given in Table 5.21 and 5.22, respectively. A brief description of the process is given below.

Purified ADN is subject to partial hydrogenation along with liquid ammonia in a fixed-bed tubular reactor. The reactor is packed with a mixture of metallic oxides selected from CoO, Mn₂O₃, P₂O₅, and Na₂O. The reaction takes place at 80°C and 20 MPa with a catalyst space velocity of 0.248 g ADN/g Cat. /hr. The resulting reactor effluent is cooled and flashed to remove most of hydrogen and a small amount of NH₃, which is compressed and recycled to the reactor. The liquid is subjected to a series of three distillation columns to recover remaining NH₃. Ethanol is used in the distillation to low the bottom temperatures in the columns so that undesirable polymerization can be avoided. The crude HMDA is then further distilled in the next three columns in series to separate purified HMDA and ACPN.

Cyclization of ACPN carried out in a fixed-bed column reactor packed with TiO₂. The reaction takes place at 220°C and 10 MPa in the presence of ethanol and water. The reactor effluent is distilled to remove NH₃ along with small amounts of ethanol and water. The crude CAPM is further distilled to remove ethanol/water mixture and heavy ends. The distilled CAPM is subjected to treatment with hydrogen and acidic ion exchange resin before final distillation to produce purified CAPM. The overall yield of this process is 41.2% to HMDA and 42.3% to CAPM based on butadiene.

Economics

Capital investment summary for this process is given in Table 5.23, and those for operation sections are listed in Table 5.24. At a capacity of 330 million lb/yr (150,000 t/yr), the process requires \$97.9 million for the battery limits and \$322.2 million for total fixed capital.

The production costs are summarized in Table 5.25. With a unit price of ADN at 58 ¢/lb and HMDA credited at 93 ¢/lb, the cash cost and the plant gate cost for CAPM are estimated at 52.9 ¢/lb and 62.7 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 96.1 ¢/lb.

Table 5.21
CAPROLACTAM AND HMDA FROM ADN
BY HYDROGENATION AND CYCLIZATION

UTILITIES SUMMARY

CAPACITY: 330 MILLION LB/YR (150,000 T/YR)
 CAPM
 AT 0.90 STREAM FACTOR

UNITS	BATTERY LIMITS	SECTION	SECTION
	TOTAL	100	200
AVERAGE CONSUMPTIONS			
COOLING WATER	GPM	39,221	24,530
PROCESS WATER	GPM	57	--
ELECTRICITY	KW	1,115	411
STEAM, 100 PSIG	M LB/HR	7	7
STEAM, 150 PSIG	M LB/HR	31	4
STEAM, 250 PSIG	M LB/HR	82	40
STEAM, 300 PSIG	M LB/HR	15	15
STEAM, 450 PSIG	M LB/HR	44	44
STEAM, 600 PSIG	M LB/HR	330	221
STEAM, 1200 PSIG	M LB/HR	399	--
REFRIGERATION, 20°F	TONS	23,888	8,096
			15,792

Table 5.22
CAPROLACTAM AND HMDA FROM ADN
BY HYDROGENATION AND CYCLIZATION

MAJOR EQUIPMENT

CAPACITY: 330 MILLION LB/YR (150,000 T/YR)
 CAPM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101	HYDROGENATION REACTOR	26.5 FT DIA 40 FT T-T	CLADDING: 316 SS PACKING: COBALT CATALYST	EQUIPPED WITH 4325 TUBES OF 3 IN OD AND 27 FT LONG
R-201	CYCLIZATION REACTOR	7.2 FT DIA 122 FT T-T	CLADDING: 316 SS PACKING: TITANIUM OXIDE	107 FT OF PACKING
R-202	HYDROGEN TREATMENT RE	2.8 FT DIA 50 FT T-T	CLADDING: 316 SS PACKING: SILICA GEL	44 FT OF PACKING
COLUMNS				
C-101	AMMONIA STRIPPER	10 FT DIA 34 FT	CLADDING: 304 SS TRAYS: 316 SS	7 VALVE TRAYS, 24 INCH SPACING
C-102	SECONDARY NH3 COLUMN	4.9 FT DIA 30 FT	CLADDING: 304 SS TRAYS: C.S.	10 VALVE TRAYS, 24 INCH SPACING
C-103	ETHANOL COLUMN	7.1 FT DIA 60 FT	CLADDING: 304 SS TRAYS: 316 SS	23 VALVE TRAYS, 24 INCH SPACING
C-104	CRDUE HMDA COLUMN	8 FT DIA 112 FT	CLADDING: 316 SS TRAYS: 316 SS	48 VALVE TRAYS, 24 INCH SPACING
C-105	HMDA COLUMN	2.8 FT DIA 54 FT	CLADDING: 316 SS TRAYS: 316 SS	24 VALVE TRAYS, 24 INCH SPACING
C-106	ACPN COLUMN	5.9 FT DIA 60 FT	CLADDING: 316 SS TRAYS: 316 SS	24 VALVE TRAYS, 24 INCH SPACING
C-201	AMMONIA STRIPPER	4.2 FT DIA 44 FT	CLADDING: 304 SS TRAYS: 316 SS	18 VALVE TRAYS, 24 INCH SPACING
C-202A,B	ETHANOL COLUMNS	11 FT DIA 88 FT	CLADDING: 316 SS TRAYS: 316 SS	28 VALVE TRAYS, 24 INCH SPACING
C-203	CRUDE CAPM COLUMN	8 FT DIA 116 FT	CLADDING: 316 SS TRAYS: 316 SS	50 VALVE TRAYS, 24 INCH SPACING
C-204A,B	ION EXCHANGE COLUMN	2.6 FT DIA 32 FT	CLADDING: 316 SS PACKING: SILICA GEL	26 FT OF PACKING ONE SPARE
C-205	DEHYDRATION COLUMN	2 FT DIA 26 FT	CLADDING: 316 SS TRAYS: 316 SS	12 VALVE TRAYS, 18 INCH SPACING
C-206	LIGHT ENDS COLUMN	1 FT DIA 45 FT	CLADDING: 316 SS TRAYS: 316 SS	36 VALVE TRAYS, 12 INCH SPACING
C-207	CAPM COLUMN	5.7 FT DIA 53 FT	CLADDING: 316 SS TRAYS: 316 SS	21 VALVE TRAYS, 24 INCH SPACING
COMPRESSORS				
K-101A,B	HYDROGEN COMPRESSOR	260 BHP	C.S.	
K-201A,B	HYDROGEN COMPRESSOR	15 BHP	C.S.	
HEAT EXCHANGERS				
E-101	PREHEATER	400 SQ FT 6.29 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-102	COOLER	4,790 SQ FT 13.79 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-103	CONDENSER	8,240 SQ FT 97.16 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-104	REBOILER	8,470 SQ FT 102.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-105	CONDENSER	2,760 SQ FT 19.42 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-106	REBOILER	2,110 SQ FT 20.39 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	

Table 5.22 (Continued)
CAPROLACTAM AND HMDA FROM ADN
BY HYDROGENATION AND CYCLIZATION

MAJOR EQUIPMENT

CAPACITY: 330 MILLION LB/YR (150,000 T/YR)
 CAPM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONCLUDED)				
E-107	CONDENSER	9,650 SQ FT 33.25 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-108	REBOILER	3,120 SQ FT 34.91 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-109	CONDENSER	3,500 SQ FT 32.21 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-110	REBOILER	3,100 SQ FT 33.82 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-111	CONDENSER	340 SQ FT 3.51 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-112	REBOILER	220 SQ FT 3.69 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-113	CONDENSER	1,050 SQ FT 15.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-114	REBOILER	1,770 SQ FT 16.27 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-115	CONDENSER	810 SQ FT 17.39 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-201	PREHEATER	3,860 SQ FT 79.04 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-202	CONDENSER	5,500 SQ FT 17.96 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-203	REBOILER	2,220 SQ FT 35.14 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-204A,B	CONDENSER	7,220 SQ FT 94.75 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-205A,B	REBOILER	5,640 SQ FT 104.2 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-206	CONDENSER	200 SQ FT 0.71 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-207	CONDENSER	550 SQ FT 9.82 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-208	REBOILER	1,880 SQ FT 10.82 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-209	COOLER	100 SQ FT 0.69 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-210	CONDENSER	380 SQ FT 1.62 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-211	REBOILER	860 SQ FT 1.79 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-212	CONDENSER	25 SQ FT 0.15 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-213	REBOILER	15 SQ FT 0.16 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-214	CONDENSER	830 SQ FT 12.98 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-215	REBOILER	1,390 SQ FT 14.28 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
TANKS				
T-101	ADIPONITRILE TANK	214,000 GAL	316 SS	
T-102	HMDA TANK	165,000 GAL	316 SS	
T-151A-C	HMDA STORAGE	275,000 GAL	316 SS	
T-152A-C	ADIPONITRILE STORAGE	520,000 GAL	316 SS	
T-201	ACPN TANK	73,000 GAL	316 SS	

Table 5.22 (Concluded)
CAPROLACTAM AND HMDA FROM ADN
BY HYDROGENATION AND CYCLIZATION

MAJOR EQUIPMENT

CAPACITY: 330 MILLION LB/YR (150,000 T/YR)
 CAPM
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
TANKS (CONCLUDED)				
T-202	ETHANOL TANK	683,000 GAL	C.S.	
T-203	SURGE TANK	70,000 GAL	304 SS	
T-204	SURGE TANK	70,000 GAL	304 SS	
T-205	CAUSTIC SODA TANK	1,000 GAL	C.S.	
T-206	CAPM TANK	54,700 GAL	316 SS	
T-251A-C	CAPM STORAGE	257,000 GAL	316 SS	
PRESSURE VESSELS				
V-101	SEPARATOR	25,000 GAL	316 SS CLAD	
V-102	REFLUX DRUM	11,100 GAL	316 SS CLAD	
V-103	REFLUX DRUM	2,700 GAL	316 SS	
V-104	REFLUX DRUM	5,700 GAL	316 SS CLAD	
V-105	REFLUX DRUM	6,600 GAL	316 SS CLAD	
V-106	REFLUX DRUM	1,500 GAL	316 SS	
V-107	REFLUX DRUM	3,700 GAL	316 SS	
V-108	RECEIVER	4,000 GAL	316 SS	
V-201	MIXING VESSEL	39,900 GAL	316 SS CLAD	WITH 220 HP AGITATOR
V-202	REFLUX DRUM	3,300 GAL	316 SS	
V-203	REFLUX DRUM	32,100 GAL	316 SS CLAD	
V-204	REFLUX DRUM	200 GAL	316 SS	
V-205	SEPARATOR	7,500 GAL	316 SS CLAD	
V-206	MIXING VESSEL	2,900 GAL	316 SS	WITH 25 HP AGITATOR
V-207	REFLUX DRUM	500 GAL	316 SS	
V-208	REFLUX DRUM	50 GAL	316 SS	
V-209	REFLUX DRUM	3,300 GAL	316 SS	
MISCELLANEOUS EQUIPMENT				
M-101	STATIC MIXER	65 MMHG	CARBON STEEL	
M-102	VACUUM SYSTEM	65 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-103	VACUUM SYSTEM	230 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-104	VACUUM SYSTEM	380 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-201	STATIC MIXER	42500	316 SS	
M-202	VACUUM SYSTEM	10 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-203	VACUUM SYSTEM	40 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-204	VACUUM SYSTEM	230 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
SPECIAL EQUIPMENT				
S-101	THIN FILM EVAPORATOR	1240 SQFT	316 SS	WITH 125 HP DRIVE
S-201	THIN FILM EVAPORATOR	80 SQFT	CARBON STEEL	WITH 15 HP DRIVE
PUMPS				
SECTION	OPERATING	SPARES	OPERATING BHP	
100	14	11	138	
200	21	21	578	

Table 5.23
CAPROLACTAM AND HMDA FROM ADN
BY HYDROGENATION AND CYCLIZATION

TOTAL CAPITAL INVESTMENT			
CAPACITY: 330 MILLION LB/YR (150,000 T/YR)			
CAPM			
AT 0.90 STREAM FACTOR			
PEP COST INDEX: 624			
	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	6,701	0.80	0.79
COLUMNS	2,418	0.79	0.57
VESSELS & TANKS	3,680	0.70	0.58
HEAT EXCHANGERS	6,808	0.88	0.82
COMPRESSORS	599	0.76	0.76
SPECIAL EQUIPMENT	1,662	0.60	0.60
MISCELLANEOUS EQUIPMENT	334	0.50	0.40
PUMPS	776	0.51	0.39

TOTAL	22,979	0.78	0.70
DIRECT INSTALLATION COSTS	30,418	0.40	0.32
INDIRECT COSTS	17,768	0.50	0.40
UNSCHEDULED EQUIPMENT, 10%	7,116	0.56	0.45

BATTERY LIMITS, INSTALLED	78,281	0.56	0.45
CONTINGENCY, 25%	19,570	0.56	0.45

BATTERY LIMITS INVESTMENT	97,851	0.56	0.45
OFF-SITES, INSTALLED			
CLARIFIED WATER	2,096	0.74	0.74
COOLING WATER	11,923	0.95	0.92
PROCESS WATER	1,166	0.62	0.62
BOILER FEED WATER	5,075	0.53	0.50
STEAM	46,576	0.92	0.88
REFRIGERATION	52,755	0.95	0.95
TANKAGE	9,580	0.65	0.65

UTILITIES & STORAGE	129,170	0.90	0.87
GENERAL SERVICE FACILITIES	45,404	0.76	0.68
WASTE TREATMENT	4,893	0.56	0.45

TOTAL	179,467	0.86	0.81
CONTINGENCY, 25%	44,867	0.86	0.81

OFF-SITES INVESTMENT	224,334	0.86	0.81
TOTAL FIXED CAPITAL	322,185	0.77	0.69

Table 5.24
CAPROLACTAM AND HMDA FROM ADN
BY HYDROGENATION AND CYCLIZATION

CAPITAL INVESTMENT BY SECTION						
CAPACITY: 330 MILLION LB/YR (150,000 T/YR)						
CAPM						
AT 0.90 STREAM FACTOR						
PEP COST INDEX: 624						
PARTIAL HYDROGENATION OF ADIPONITRILE						
CYCLIZATION OF 6-AMINOCAPRONITRILE						
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
	UP	DOWN	UP	DOWN	UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.						
REACTORS	4,980	0.83	0.83	1,722	0.71	0.69
COLUMNS	965	0.75	0.58	1,453	0.82	0.56
VESSELS & TANKS	1,693	0.66	0.64	1,987	0.74	0.52
HEAT EXCHANGERS	3,650	0.88	0.82	3,159	0.87	0.81
COMPRESSORS	538	0.76	0.76	62	0.76	0.76
SPECIAL EQUIPMENT	1,458	0.60	0.60	204	0.60	0.60
MISCELLANEOUS EQUIPMENT	159	0.50	0.40	175	0.50	0.40
PUMPS	320	0.45	0.36	456	0.56	0.42
TOTAL	13,761	0.78	0.74	9,217	0.78	0.65
DIRECT INSTALLATION COSTS	18,036	0.39	0.32	12,381	0.41	0.32
INDIRECT COSTS	10,581	0.50	0.42	7,187	0.50	0.38
UNSCHEDULED EQUIPMENT, 10%	4,238	0.55	0.47	2,879	0.56	0.43
BATTERY LIMITS INSTALLED	46,616	0.55	0.47	31,664	0.56	0.43
CONTINGENCY, 25%	11,654	0.55	0.47	7,916	0.56	0.43
BATTERY LIMITS INVESTMENT	58,270	0.55	0.47	39,580	0.56	0.43
OFFSITES, INSTALLED						
CLARIFIED WATER	978	0.74	0.74	1,118	0.74	0.74
COOLING WATER	5,849	0.95	0.92	6,074	0.95	0.92
PROCESS WATER	561	0.62	0.62	583	0.62	0.62
BOILER FEED WATER	1,612	0.52	0.50	3,462	0.53	0.50
STEAM	15,870	0.91	0.86	30,706	0.93	0.89
REFRIGERATION	17,880	0.95	0.95	34,875	0.95	0.95
TANKAGE	6,938	0.65	0.65	2,642	0.65	0.65
UTILITIES & STORAGE	49,690	0.88	0.85	79,459	0.91	0.89

Table 5.25
CAPROLACTAM AND HMDA FROM ADN
BY HYDROGENATION AND CYCLIZATION

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			-----
AMMONIA	8.75 ¢/LB	0.0002 LB	NEGL
HYDROGEN	0.418 ¢/FT^3	20.0358 FT^3	8.37
ETHANOL	155 ¢/GALLON	0.00252 GALLON	0.39
ADIPONITRILE	58 ¢/LB	2.00416 LB	116.24
GROSS RAW MATERIALS			125.00
BY-PRODUCTS			-----
LIGHT ENDS AS FUEL	2.21 \$/MMBTU	-0.00132 MMBTU	-0.29
HMDA	93 ¢/LB	-1 LB	-93.00
TOTAL BY-PRODUCTS			-93.29
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			-----
COOLING WATER	7.45 ¢/MGAL	56.2 GAL	469 LITERS
PROCESS WATER	1.101 \$/MGAL	0.0817 GAL	0.682 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	0.906 LB	0.906 KG
STEAM, 600 PSIG	5.72 \$/MLB	11.3 LB	11.3 KG
STEAM, 1500 PSIG	6.16 \$/MLB	9.53 LB	9.53 KG
ELECTRICITY	4 ¢/KWH	0.0266 KWH	0.0588 KWH
REFRIGERATION, 20°F	5.08 ¢/TON-HR	0.571 TON-HR	4.43 KWH
TOTAL UTILITIES			16.17

Table 5.25 (Concluded)
CAPROLACTAM AND HMDA FROM ADN
BY HYDROGENATION AND CYCLIZATION

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	165	330#	660
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	71.4	97.9	143.8
OFFSITES	128.3	224.3	406.3
TOTAL FIXED CAPITAL (TFC)	199.7	322.2	550.1
SCALING EXPONENTS		0.69	0.77
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	125.00	125.00	125.00
BY-PRODUCTS	-93.29	-93.29	-93.29
UTILITIES	16.17	16.17	16.17
VARIABLE COSTS	47.88	47.88	47.88
OPERATING LABOR, 3/SHIFT, \$33.58/HR	0.53	0.27	0.13
MAINTENANCE LABOR, 3%/YR OF BLI	1.30	0.89	0.65
CONTROL LAB LABOR, 20% OF OPER LABOR	0.11	0.05	0.03
LABOR COSTS	1.94	1.21	0.81
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.30	0.89	0.65
OPERATING SUPPLIES, 10% OF OPER LABOR	0.05	0.03	0.01
TOTAL DIRECT COSTS	51.17	50.01	49.35
PLANT OVERHEAD, 80% OF LABOR COSTS	1.55	0.97	0.65
TAXES AND INSURANCE, 2%/YR OF TFC	2.42	1.95	1.67
PLANT CASH COSTS	55.14	52.93	51.67
DEPRECIATION, 10%/YR OF TFC	12.10	9.76	8.33
PLANT GATE COSTS	67.24	62.69	60.00
G&A, SALES, RESEARCH	9.00	9.00	9.00
NET PRODUCTION COST	76.24	71.69	69.00
ROI BEFORE TAXES, 25%/YR OF TFC	30.26	24.41	20.84
PRODUCT VALUE	106.50	96.10	89.84

* OF CAPM

BASE CASE

HMDA AND CAPM FROM BUTADIENE VIA ADIPONITRILE

Process Description

This integrated process is SRI's design based on patents assigned to DuPont and BASF. In the process adiponitrile (ADN) is produced from butadiene by two-step hydrocyanation process described in DuPont patents. The reactions take place in the presence of Ni catalyst. In the process, butadiene is first hydrocyanated to mainly 3-pentenenitrile (3PN) and 4-pentenenitrile (4PN) with some by-products, such as 2PN and 2-methyl-3-butenenitrile (2M3B). After removal of 2PN, and isomerization of 2M3B to 3PN, the pentenenitriles are subjected to second hydrocyanation to form ADN and some by-products. The crude ADN is purified by vacuum distillation in two columns in series to remove its isomers (e.g. 2-methylglutaronitrile, 3- methylglutaronitrile, and ethylsuccinonitrile). ADN is then subjected to partial hydrogenation to form HMDA and 6-aminocapronitrile (ACPN) as described in the previous process.

Economics

Capital investment summary for this process is given in Table 5.26. At a capacity of 330 million lb/yr (150,000 t/yr) for co-production of CAPM and HMDA at equal amounts, the process requires \$195.7 million for the battery limits and \$476.6 million for total fixed capital.

The production costs are summarized in Table 5.27. With a unit price of butadiene at 13 ¢/lb and HMDA credited at 93 ¢/lb, the cash cost and the plant gate cost for CAPM are estimated at 24.5 ¢/lb and 38.9 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 84 ¢/lb.

Table 5.26
HMDA AND CAPROLACTAM FROM BUTADIENE VIA ADN
BY HYDROCYANATION, HYDROGENATION AND CYCLIZATION

TOTAL CAPITAL INVESTMENT			
CAPACITY: 330 MILLION LB/YR (150,000 T/YR)			
HMDA AND CAPM			
AT 0.90 STREAM FACTOR			
PEP COST INDEX: 624			
CAPACITY EXPONENT			
COST (\$1,000)			

BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	14,342	0.76	0.76
COLUMNS	8,116	0.90	0.73
VESSELS & TANKS	8,090	0.74	0.57
HEAT EXCHANGERS	11,640	0.87	0.83
COMPRESSORS	599	0.76	0.76
SPECIAL EQUIPMENT	3,315	0.60	0.60
MISCELLANEOUS EQUIPMENT	862	0.55	0.51
PUMPS	1,492	0.41	0.31
-----	-----	-----	-----
TOTAL	48,457	0.79	0.70
DIRECT INSTALLATION COSTS	59,851	0.44	0.37
INDIRECT COSTS	33,989	0.53	0.44
UNSCHEDULED EQUIPMENT, 10%	14,230	0.59	0.49
-----	-----	-----	-----
BATTERY LIMITS, INSTALLED	156,528	0.59	0.49
CONTINGENCY, 25%	39,132	0.59	0.49
-----	-----	-----	-----
BATTERY LIMITS INVESTMENT	195,660	0.59	0.49
OFF-SITES, INSTALLED			
CLARIFIED WATER	2,754	0.74	0.74
COOLING WATER	16,553	0.94	0.95
PROCESS WATER	1,478	0.62	0.62
BOILER FEED WATER	5,887	0.59	0.59
STEAM	56,983	0.94	0.93
REFRIGERATION	56,498	0.95	0.95
INERT GAS	169	0.52	0.52
TANKAGE	6,193	0.65	0.65
-----	-----	-----	-----
UTILITIES & STORAGE	146,515	0.91	0.90
GENERAL SERVICE FACILITIES	68,435	0.74	0.65
WASTE TREATMENT	9,783	0.59	0.49
-----	-----	-----	-----
TOTAL	224,732	0.85	0.80
CONTINGENCY, 25%	56,183	0.85	0.80
-----	-----	-----	-----
OFF-SITES INVESTMENT	280,916	0.85	0.80
TOTAL FIXED CAPITAL	476,575	0.75	0.67

Table 5.27
HMDA AND CAPROLACTAM FROM BUTADIENE VIA ADN
BY HYDROCYANATION, HYDROGENATION AND CYCLIZATION

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
BUTADIENE	13 ¢/LB	1.13112 LB	14.70
AMMONIA	8.75 ¢/LB	0.00364 LB	0.03
HYDROGEN (97%)	0.388 ¢/FT^3	20.0358 FT^3	7.77
ETHANOL	155 ¢/GALLON	0.00252 GALLON	0.39
HYDROGEN CYANIDE	46.18 ¢/LB	1.12652 LB	52.02
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.00712 LB	1.99
SODIUM BISULFITE	19.25 ¢/LB	0.22824 LB	4.39
SODIUM SULFITE	30.5 ¢/LB	0.13854 LB	4.23
TRIPHENYLBORANE	10.26 \$/LB	0.00026 LB	0.27
PHOSPHORUS TRICHLORIDE	49 ¢/LB	0.0004 LB	0.02
CYCLOHEXANE	15.62 ¢/LB	0.00122 LB	0.02
NICKEL POWDER	8.79 \$/LB	0.00082 LB	0.72
GROSS RAW MATERIALS			86.55
BY-PRODUCTS			
LIGHT ENDS AS FUEL	2.21 \$/MMBTU	-0.00132 MMBTU	-0.29
HMDA	93 ¢/LB	-1 LB	-93.00
TOTAL BY-PRODUCTS			-93.29
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	95.2 GAL	0.71
PROCESS WATER	1.101 \$/MGAL	0.387 GAL	0.04
STEAM, 150 PSIG	4.51 \$/MLB	4.78 LB	2.15
STEAM, 600 PSIG	5.72 \$/MLB	15 LB	8.58
STEAM, 1500 PSIG	6.16 \$/MLB	9.53 LB	5.87
ELECTRICITY	4 ¢/KWH	0.102 KWH	0.41
NATURAL GAS	3.24 \$/MMBTU	167 BTU	0.05
INERT GAS, LOW P	0.51 \$/MSCF	0.263 SCF	0.01
REFRIGERATION, 20°F	5.08 ¢/TON-HR	0.571 TON-HR	2.90
REFRIGERATION, 40°F	5 ¢/TON-HR	0.044 TON-HR	0.22
TOTAL UTILITIES			20.94

Table 5.27 (Concluded)
HMDA AND CAPROLACTAM FROM BUTADIENE VIA ADN
BY HYDROCYANATION, HYDROGENATION AND CYCLIZATION

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	165	330#	660
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	139.1	195.7	294.4
OFFSITES	160.9	280.9	505.4
TOTAL FIXED CAPITAL (TFC)	299.9	476.6	799.8
SCALING EXPONENTS		0.67	0.75
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	86.55	86.55	86.55
BY-PRODUCTS	-93.29	-93.29	-93.29
UTILITIES	20.94	20.94	20.94
VARIABLE COSTS	14.20	14.20	14.20
OPERATING LABOR, 12/SHIFT, \$33.58/HR	2.14	1.07	0.53
MAINTENANCE LABOR, 3%/YR OF BLI	2.53	1.78	1.34
CONTROL LAB LABOR, 20% OF OPER LABOR	0.43	0.21	0.11
LABOR COSTS	5.10	3.06	1.98
MAINTENANCE MATERIALS, 3%/YR OF BLI	2.53	1.78	1.34
OPERATING SUPPLIES, 10% OF OPER LABOR	0.21	0.11	0.05
TOTAL DIRECT COSTS	22.04	19.15	17.57
PLANT OVERHEAD, 80% OF LABOR COSTS	4.08	2.45	1.58
TAXES AND INSURANCE, 2%/YR OF TFC	3.64	2.89	2.42
PLANT CASH COSTS	29.76	24.49	21.57
DEPRECIATION, 10%/YR OF TFC	18.18	14.44	12.12
PLANT GATE COSTS	47.94	38.93	33.69
G&A, SALES, RESEARCH	9.00	9.00	9.00
NET PRODUCTION COST	56.94	47.93	42.69
ROI BEFORE TAXES, 25%/YR OF TFC	45.45	36.10	30.29
PRODUCT VALUE	102.39	84.03	72.98

* OF HMDA AND CAPM
BASE CASE

NYLON 6 BY HYDROLYTIC POLYMERIZATION

Process Description

Figure 5.5 (foldout at end of report) presents the flow diagram for this process, and the utilities summary and major equipment list are given in Table 5.28 and 5.29, respectively. A brief description of the process is given below.

The process shown below is based on patents assigned to BASF, Mitsubishi Chemical, and Unitika. Polymerization of caprolactam, mixed with aqueous acetic acid, is conducted continuously in a reactor at 270-280°C and 1.22 atm. The polymer is pumped into an extruder. The polymer strands from the extruder are quenched in water and cut into chips. The chip slurry feeds an extraction column where the chips are extracted with hot water to remove oligomer and unreacted monomer. Water leaving the column goes to monomer recovery. The extracted nylon 6 chips are reslurried in water and feed a drying column. The chips are dried mechanically by a rotating screen and thermally by hot nitrogen (190°C). The dried nylon 6 chips are cooled and transferred to storage bins for bagging or bulk shipment. The depolymerization process for nylon 6 scrap and oligomer is approximately the same as that shown in the Yearbook as Nylon 6 Melt from Caprolactam for Direct Spinning". Product yield on caprolactam and waste nylon is 98.8%.

Economics

Capital investment summary for this process is given in Table 5.30, and those for operation sections are listed in Table 5.31. At a capacity of 135 million lb/yr (61,200 t/yr), the process requires \$52.3 million for the battery limits and \$90.5 million for total fixed capital.

The production costs are summarized in Table 5.32. With a unit price of CAPM at 90 ¢/lb, the cash cost and the plant gate cost for nylon 6 chips are estimated at 100.7 ¢/lb and 107.4 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 136.2 ¢/lb.

Table 5.28
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

UTILITIES SUMMARY				
	UNITS	BATTERY LIMITS TOTAL	SECTION 100	SECTION 200
AVERAGE CONSUMPTIONS				
COOLING WATER	GPM	7,275	1,421	5,854
PROCESS WATER	GPM	10	10	--
ELECTRICITY	KW	2,502	2,226	276
NATURAL GAS	MM BTU/HR	4	3	1
INERT GAS, LOW P	M SCF/HR	2	1	1
STEAM, 50 PSIG	M LB/HR	18	10	8
STEAM, 300 PSIG	M LB/HR	5	5	--
STEAM, 600 PSIG	M LB/HR	15	--	15
STEAM, 1500 PSIG	M LB/HR	66	--	66

Table 5.29
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

MAJOR EQUIPMENT

CAPACITY: 135 MILLION LB/YR (61,200 T/YR)
 NYLON 6 CHIPS
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101	POLYMERIZER	49,968.2 GAL	CLADDING: 316 SS AGITATOR: 304 SS	UPPER PART 8.4FT X 13FT, LOWER PART 6FT X 71FT, AND WITH 65 HP AGITATOR
R-201	DEPOLYMERIZER	3,233.24 GAL	SHELL: 316 SS AGITATOR: 316 SS	JACKETED, WITH 18 HP TURBINE AGITATOR
COLUMNS				
C-101	EXTRACTION COLUMN	11.5 FT DIA 75 FT	CLADDING: 316 SS PACKING: PORCELAIN	50 FT OF 1 INCH RING PACKING WITH 50 FT RING PACKING
C-102	DRYING COLUMN	13 FT DIA 83 FT	CLADDING: 316 SS TRAYS: C.S.	12 VALVE TRAYS, 24 INCH SPACING WITH 10 HP AGITATOR ON THE TOP
C-201	CONCENTRATION COLUMN	5.5 FT DIA 28 FT	CLADDING: 316 SS PACKING: 316 SS	20 FT OF 1 INCH RING PACKING
C-202A,B	ABSORBERS	4.5 FT DIA 11 FT	CLADDING: 316 SS PACKING: ACTIVATED CARBON	8 FT OF PACKING
C-203	DEWATERING COLUMN	5.5 FT DIA 28 FT	SHELL: 316 SS PACKING: 316 SS	20 FT OF 1 INCH RING PACKING
C-204	MONOMER REFINING COLUMN	5.5 FT DIA 24 FT	SHELL: 316 SS PACKING: 316 SS	15 FT OF 1 INCH RING PACKING
COMPRESSORS				
K-101A,B	NITROGEN BLOWER	1,469.65 BHP	C.S.	
HEAT EXCHANGERS				
E-101	PREHEATER	73.4827 SQ FT 0.22 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-102	CONDENSER	29.3931 SQ FT 0.06 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-103	COOLER	710.333 SQ FT 1.63 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-104	PREHEATER	122.471 SQ FT 0.86 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-105	CONDENSER	8,009.62 SQ FT 3.06 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-106	HEATER	2,008.53 SQ FT 1.73 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-201	CONDENSER	1,959.54 SQ FT 14.24 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-202	REBOILER	2,400.44 SQ FT 14.72 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-203	CONDENSER	36.7414 SQ FT 0.35 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-204	CONDENSER	563.367 SQ FT 5.25 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-205	CONDENSER	906.287 SQ FT 3.68 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-206	REBOILER	2,106.5 SQ FT 3.98 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-207	CONDENSER	244.942 SQ FT 0.38 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-208	REBOILER	171.46 SQ FT 0.4 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	

Table 5.29 (Concluded)
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

MAJOR EQUIPMENT

CAPACITY: 135 MILLION LB/YR (61,200 T/YR)
 NYLON 6 CHIPS
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
PROCESS FURNACES				
F-101	DOWTHERM	2.20448 MMBTU/HR	C.S.	FOR R-101, NOT SHOWN IN FLOW DIAGRAM
F-201	DOWTHERM	1 MMBTU/HR	C.S.	FOR R-201 & V-204, NOT SHOWN IN FLOW DIAGRAM
TANKS				
T-101A,B	CAPROLACTAM TANK	37,476.2 GAL	316 SS	WITH HEATING COILS
T-151	CAPROLACTAM SOTRAGE	374,762 GAL	316 SS	WITH HEATING COILS; NOT SHOWN IN FLOW DIAGRAM
T-201	CAPM SOLUTION TANK	23,759.4 GAL	316 SS	WITH 65 HP AGITATOR
PRESSURE VESSELS				
V-101	MIXING VESSEL	440.896 GAL	316 SS	WITH 2 HP AGITATOR AND JACKETED
V-102	GEED VESSEL	440.896 GAL	316 SS	WITH 2 HP AGITATOR AND JACKETED
V-103	REFLUX DRUM	48.9885 GAL	316 SS	
V-104	WATER SURGE VESSEL	2,008.53 GAL	316 SS	
V-105	RECYCLE LIQUID VESSEL	2,596.39 GAL	316 SS	
V-106	WATER SEPARATOR	2,449.42 GAL	C.S.	
V-201	REFLUX DRUM	1,935.04 GAL	C.S.	
V-202	OLIGOMER SURGE VESSEL	1,469.65 GAL	316 SS	
V-203	PHOSPHORIC ACID VESSEL	661.344 GAL	316 SS	
V-204A,B	MELTING VESSELS	1,102.24 GAL	316 SS	EACH EQUIPPED WITH 15 HP TURBINE AGITATOR
V-205	CAUSTIC VESSEL	734.827 GAL	316 SS	
V-206A,B	RECOVD MONOMER TREATMN	9,797.7 GAL	316 SS CLAD	EACH EQUIPPED WITH 40 HP TURBINE AGITATOR
V-207	RELUX DRUM	563.367 GAL	316 SS	
V-208	RELUX DRUM	220.448 GAL	316 SS	
MISCELLANEOUS EQUIPMENT				
M-101	WEIGH SCALE	200 LB DIAL	CARBON STEEL	
M-102	STATIC MIXER	7900 LB/HR	CARBON STEEL	
M-201	NYLON 6 SCRAP HOPPER	130 CUFT	ALUMINUM	
M-202	WEIGH SCALE	50 LB DIAL	ALUMINUM	
M-203A,B	FILTERS	4300 LB/HR	ALUMINUM	CARTRIDGE FILTER
M-204	VACUUM SYSTEM	30 MMHG	ALUMINUM	NOT SHOWN IN FLOW DIAGRAM
M-205	VACUUM SYSTEM	150 MMHG	ALUMINUM	NOT SHOWN IN FLOW DIAGRAM
M-206	VACUUM SYSTEM	5 MMHG	ALUMINUM	NOT SHOWN IN FLOW DIAGRAM
SPECIAL EQUIPMENT				
S-101	EXTRUDER	8000 IB/HR	316 SS	
S-102	QUENCHER	8000 IB/HR	316 SS	
S-103	PELLETIZER	8000 IB/HR	316 SS	
S-201	EVAPORATOR	170 SQFT	CARBON STEEL	THIN FILM EVAPOATOR, WITH 25 HP DRIVE
PACKAGE UNITS				
G-101A-D	STORAGE BINS	5400 CUFT	EXPOXY LINED	
G-102	LOADING AND PACKAGING	150 BAGS/HR	CARBON STEEL	
G-103	CONVEYING SYSTEM	8000 LB/HR	ALUMINUM	
PUMPS				
SECTION	OPERATING	SPARES	OPERATING BHP	
100	10	9	35	
200	17	15	19	

Table 5.30
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

TOTAL CAPITAL INVESTMENT			
CAPACITY: 135 MILLION LB/YR (61,200 T/YR)			
NYLON 6 CHIPS			
AT 0.90 STREAM FACTOR			
PEP COST INDEX: 624			
	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	887	0.66	0.65
COLUMNS	2,118	0.79	0.64
VESSELS & TANKS	1,736	0.57	0.60
HEAT EXCHANGERS	843	0.81	0.73
FURNACES	138	0.75	0.75
COMPRESSORS	2,005	0.76	0.76
SPECIAL EQUIPMENT	3,340	0.67	0.66
MISCELLANEOUS EQUIPMENT	157	0.63	0.62
PUMPS	312	0.23	0.17

TOTAL	11,536	0.69	0.65
DIRECT INSTALLATION COSTS	14,532	0.46	0.37
PACKAGE UNIT	1,425	0.57	0.47
INDIRECT COSTS	10,537	0.52	0.44
UNSCHEDULED EQUIPMENT, 10%	3,803	0.55	0.47

BATTERY LIMITS, INSTALLED	41,834	0.55	0.47
CONTINGENCY, 25%	10,459	0.55	0.47

BATTERY LIMITS INVESTMENT	52,293	0.55	0.47
OFF-SITES, INSTALLED			
CLARIFIED WATER	386	0.40	0.40
COOLING WATER	1,393	0.92	0.92
PROCESS WATER	241	0.40	0.40
BOILER FEED WATER	1,623	0.40	0.40
STEAM	7,572	0.73	0.73
INERT GAS	77	0.40	0.40
TANKAGE	1,189	0.65	0.65
WAREHOUSE FACILITIES	2,126	0.60	0.60

UTILITIES & STORAGE	14,608	0.68	0.66
GENERAL SERVICE FACILITIES	13,380	0.58	0.51
WASTE TREATMENT	2,615	0.55	0.47

TOTAL	30,604	0.63	0.58
CONTINGENCY, 25%	7,651	0.63	0.58

OFF-SITES INVESTMENT	38,254	0.63	0.58
TOTAL FIXED CAPITAL	90,547	0.58	0.52

Table 5.31
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

CAPITAL INVESTMENT BY SECTION

CAPACITY: 135 MILLION LB/YR (61,200 T/YR)
 NYLON 6 CHIPS
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	POLYMERIZATION			MONOMER RECOVERY SECTION		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.						
REACTORS	732	0.67	0.67	155	0.58	0.54
COLUMNS	1,338	0.71	0.59	781	0.92	0.72
VESSELS & TANKS	782	0.62	0.73	954	0.52	0.50
HEAT EXCHANGERS	270	0.79	0.55	573	0.82	0.81
FURNACES	93	0.78	0.78	45	0.70	0.70
COMPRESSORS	2,005	0.76	0.76	--	--	--
SPECIAL EQUIPMENT	2,626	0.65	0.65	714	0.75	0.72
MISCELLANEOUS EQUIPMENT	20	0.53	0.52	137	0.64	0.63
PUMPS	141	0.28	0.20	171	0.18	0.15
TOTAL	8,008	0.69	0.66	3,529	0.71	0.63
DIRECT INSTALLATION COSTS	9,978	0.53	0.45	4,554	0.27	0.22
PACKAGE UNIT	1,425	0.57	0.47	--	--	--
INDIRECT COSTS	7,439	0.55	0.49	3,098	0.43	0.33
UNSCHEDULED EQUIPMENT, 10%	2,685	0.59	0.52	1,118	0.47	0.37
BATTERY LIMITS INSTALLED	29,536	0.59	0.52	12,299	0.47	0.37
CONTINGENCY, 25%	7,384	0.59	0.52	3,075	0.47	0.37
BATTERY LIMITS INVESTMENT	36,920	0.59	0.52	15,373	0.47	0.37
OFFSITES, INSTALLED						
CLARIFIED WATER	81	0.40	0.40	304	0.40	0.40
COOLING WATER	272	0.92	0.92	1,121	0.92	0.92
PROCESS WATER	46	0.40	0.40	188	0.40	0.40
BOILER FEED WATER	314	0.40	0.40	1,310	0.40	0.40
STEAM	975	0.60	0.60	6,597	0.75	0.75
INERT GAS	39	0.40	0.40	39	0.40	0.40
TANKAGE	1,189	0.65	0.65	--	--	--
WAREHOUSE FACILITIES	2,126	0.60	0.60	--	--	--
UTILITIES & STORAGE	5,042	0.61	0.61	9,559	0.71	0.69

Table 5.32
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
CAPROLACTAM	90 ¢/LB	0.94769 LB	85.29
NYLON 6 SCRAP	64.5 ¢/LB	0.06493 LB	4.19
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
CAUSTIC SODA	11 ¢/LB	0.00373 LB	0.04
OTHER CHEMICALS	1 ¢/LB	0.02 LB	0.02
GROSS RAW MATERIALS			89.75
UTILITIES			
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
COOLING WATER	7.45 ¢/MGAL	25.5 GAL	213 LITERS
PROCESS WATER	1.101 \$/MGAL	0.0343 GAL	0.287 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	1.07 LB	1.07 KG
STEAM, 600 PSIG	5.72 \$/MLB	1.17 LB	1.17 KG
STEAM, 1500 PSIG	6.16 \$/MLB	3.86 LB	3.86 KG
ELECTRICITY	4 ¢/KWH	0.146 KWH	0.322 KWH
NATURAL GAS	3.24 \$/MMBTU	250 BTU	139 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.143 SCF	8.93 LITERS
TOTAL UTILITIES			4.39

Table 5.32 (Concluded)
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	68	135#	270
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	37.6	52.3	76.7
OFFSITES	25.6	38.3	59.1
TOTAL FIXED CAPITAL (TFC)	63.2	90.6	135.8
SCALING EXPONENTS	0.52	0.58	
PRODUCTION COSTS (¢/LB)			
RAW MATERIALS	89.75	89.75	89.75
UTILITIES	4.39	4.39	4.39
VARIABLE COSTS	94.14	94.14	94.14
OPERATING LABOR, 4/SHIFT, \$33.58/HOUR	1.74	0.87	0.44
MAINTENANCE LABOR, 3%/YR OF BLI	1.67	1.16	0.85
CONTROL LAB LABOR, 20% OF OPER LABOR	0.35	0.17	0.09
LABOR COSTS	3.76	2.20	1.38
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.67	1.16	0.85
OPERATING SUPPLIES, 10% OF OPER LABOR	0.17	0.09	0.04
TOTAL DIRECT COSTS	99.74	97.59	96.41
PLANT OVERHEAD, 80% OF LABOR COSTS	3.01	1.76	1.10
TAXES AND INSURANCE, 2%/YR OF TFC	1.87	1.34	1.01
PLANT CASH COSTS	104.62	100.69	98.52
DEPRECIATION, 10%/YR OF TFC	9.37	6.71	5.03
PLANT GATE COSTS	113.99	107.40	103.55
G&A, SALES, RESEARCH	12.00	12.00	12.00
NET PRODUCTION COST	125.99	119.40	115.55
ROI BEFORE TAXES, 25%/YR OF TFC	23.43	16.77	12.57
PRODUCT VALUE	149.42	136.17	128.12

* OF NYLON 6 CHIPS

BASE CASE

6 ECONOMICS FOR NYLON 66 AND ITS PRECURSORS

INTRODUCTION

In this section, we present economics for the production of nylon 66 resin and its precursors. Also presented are flow diagrams for these processes along with brief process descriptions.

COMMERCIAL PROCESSES FOR THE PRODUCTION OF ADIPIC ACID

Adipic acid (ADA) is produced by oxidation of KA oil (a mixture of cyclohexanone and cyclohexanol), which is prepared either from cyclohexane by oxidation or from phenol by hydrogenation. At the present, majority of ADA production is based on the cyclohexane route. Recently, cyclohexanol is produced from benzene via cyclohexene by partial hydrogenation. The latter is subjected to hydration to produce cyclohexanol, which is then oxidized to ADA similarly as the conventional process. There have been many activities in research development on various processes producing ADA from butadiene. SRI has reviewed these activities in both PEP Report 3B and the present report. Among those processes, we believe that a process, which produces ADA from butadiene by carboalkoxylation, is more commercially viable. In this section we present the following three processes for the production of ADA.

- Adipic acid from cyclohexane by the oxidation process
- Adipic acid from butadiene by the carboalkoxylation process
- Adipic acid from benzene by the partial hydrogenation process

ADIPIC ACID FROM CYCLOHEXANE BY THE OXIDATION PROCESS

Process Description

Figure 6.1 (foldout at end of report) presents the flow diagram for the oxidation process, and the utilities summary and major equipment list are given in Table 6.1 and 6.2, respectively. The following is a brief description of the process.

The continuous process described below is SRI's process modified from the earlier version with design based on current patents reviewed in PEP report 3B.

Modification involves with selectivity to KA oil improved to 85%, recovery of dicarboxylic acids from the caustic wash stream, and treatment of unabsorbed off-gas.

Cyclohexane is oxidized in 4 cascaded, agitated, jacket cooled autoclave at 10 atm and 160°C in the presence of Co-naphthenate catalyst. Reactor effluent passes to a peroxide converter, where cyclohexylperoxide is converted to KA oil. The resulting mixture is neutralized and washed with caustic solution. The aqueous caustic solution is treated with sulfuric acid to recover dicarboxylic acids as by-products. The washed organic stream is distilled in two columns in series for recovery of cyclohexane, which is recycled to oxidation operation. The bottom stream from the second distillation column contains some esters, which is removed by hydrolyzing with aqueous caustic and extracting with water. The extracted KA oil still contains some heavy ends, which is separated from KA oil by evaporating the latter. The evaporation residue is incinerated.

The purified KA oil is oxidized with nitric acid at 1 atm and 70°C. The reactor effluent is air stripped to remove gas products, which is absorbed with water to recover nitric oxide as a nitric acid solution and recycled to the nitric oxidation operation. The unabsorbed nitrous oxide is catalytically converted to a mixture of nitrogen and oxygen, which is cooled and vented to atmosphere. The stripped crude adipic acid is purified through two steps of crystallization, centrifuging, and washing before the purified adipic acid is dried in a rotary dryer. Overall yield of adipic acid is 80.2%.

Cost Estimates

Capital investment summary for this process is given in Table 6.3, and those for operation sections are listed in Table 6.4. At a capacity of 300 million lb/yr (136,000 t/yr), the process requires \$158.2 million for the battery limits and \$251.9 million for total fixed capital.

The production costs are summarized in Table 6.5. With a unit price of cyclohexane at 15.62 ¢/lb, the cash cost and the plant gate cost for ADA are estimated at 34.7 ¢/lb and 43.1 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 71.1 ¢/lb.

Table 6.1
ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

UTILITIES SUMMARY

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

UNITS	BATTERY LIMITS	SECTION	SECTION	SECTION	SECTION	SECTION	SECTION
	TOTAL	100	200	300	400	500	600
<hr/>							
AVERAGE CONSUMPTIONS							
COOLING WATER	GPM	36,029	1,630	11,519	14,355	6,257	2,204
ELECTRICITY	KW	1,931	731	248	256	625	50
NATURAL GAS	MM BTU/HR	0	--	--	0	--	--
INERT GAS, LOW P	M SCF/HR	13	6	--	--	--	7
STEAM, 100 PSIG	M LB/HR	406	--	98	298	7	1
STEAM, 150 PSIG	M LB/HR	68	13	25	--	--	29
STEAM, 300 PSIG	M LB/HR	1	--	--	--	--	1
STEAM, 600 PSIG	M LB/HR	45	45	--	--	--	--
STEAM, 100 PSIG	M LB/HR	-45	-45	--	--	--	--
STEAM, 600 PSIG	M LB/HR	-7	--	--	-7	--	--
REFRIGERATION, 40°F	TONS	133	105	--	--	--	28

Table 6.2
ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
ADIPIC ACID
AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101	OXIDATION REACTOR	22,000 GAL	CLADDING: 304 SS AGITATOR: 316 SS	WITH 160 HP AGITATOR, AND JACKETED
R-102	OXIDATION REACTOR	22,000 GAL	CLADDING: 304 SS AGITATOR: 316 SS	WITH 160 HP AGITATOR, AND JACKETED
R-103	OXIDATION REACTOR	22,000 GAL	CLADDING: 304 SS AGITATOR: 316 SS	WITH 160 HP AGITATOR, AND JACKETED
R-104	OXIDATION REACTOR	22,000 GAL	CLADDING: 304 SS AGITATOR: 316 SS	WITH 160 HP AGITATOR, AND JACKETED
R-105	OXIDATION REACTOR	22,000 GAL	CLADDING: 304 SS AGITATOR: 316 SS	WITH 160 HP AGITATOR, AND JACKETED
R-301 R-302A,B	OXIDATION REACTOR N ₂ O DECOMPOSERS	15,000 GAL 12,460 SQ FT 18.7 MMBTU/HR	CLADDING: 304 SS SHELL: C.S. TUBES: C.S.	860 TUBES OF 2.5 IN DIA. AND 25 FT
COLUMNS				
C-101	COOLING SCRUBBER	5.8 FT DIA 26 FT	SHELL: 304 SS PACKING: 316 SS	14 FT OF 2 INCH RING PACKING
C-102	STRIPPING COLUMN	5.8 FT DIA 26 FT	SHELL: 304 SS PACKING: 316 SS	12 FT OF 2 INCH RING PACKING
C-201	DISTILLATION COLUMN	12 FT DIA 48 FT	SHELL: 304 SS TRAYS: 316 SS	15 SIEVE TRAYS, 24 INCH SPACING
C-202	DISTILLATION COLUMN	7.5 FT DIA 44 FT	SHELL: 304 SS TRAYS: 316 SS	16 SIEVE TRAYS, 24 INCH SPACING
C-203	EXTRACTION COLUMN	6 FT DIA 30 FT	SHELL: 304 SS TRAYS: 316 SS	10 SIEVE TRAYS, 24 INCH SPACING 10 ROTARY DISCS AND 25 HP DRIVE
C-301	DEGASSING COLUMN	6 FT DIA 36 FT	SHELL: 304 SS PACKING: 316 SS	20 FT OF 2 INCH RING PACKING
C-302	NOX ABSORBER	10 FT DIA 70 FT	SHELL: 316 SS PACKING: 316 SS	58 FT OF 2 INCH RING PACKING
C-303A,B	DISTILLATION COLUMN	16 FT DIA 80 FT	SHELL: 316 SS TRAYS: 316 SS	32 SIEVE TRAYS, 24 INCH SPACING
C-501	STRIPPING COLUMN	2 FT DIA 16 FT	SHELL: 316 SS TRAYS: 316 SS	3 SIEVE TRAYS, 24 INCH SPACING
C-502	DISTILLATION COLUMN	2 FT DIA 42 FT	SHELL: 316 SS TRAYS: 316 SS	16 SIEVE TRAYS, 24 INCH SPACING
C-601	DIBASIC ACID COLUMN	6.3 FT DIA 64 FT	SHELL: 316 SS TRAYS: 304 SS	36 SIEVE TRAYS, 18 INCH SPACING
COMPRESSORS				
K-101A,B K-301A,B K-401A,B	AIR COMPRESSOR AIR BLOWER AIR BLOWER	2,840 BHP 15 BHP 30 BHP	C.S. C.S. C.S.	STEAM TURBINE WITH 600 PSIG STEAM, ONE SPARE CENTRIFUGAL, ONE SPARE CENTRIFUGAL, ONE SPARE
HEAT EXCHANGERS				
E-101	COOLER	130 SQ FT 1.1 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	WITH 40°F CHILLED WATER COOLING
E-102	COOLER	40 SQ FT 0.16 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	WITH 40°F CHILLED WATER COOLING
E-103	HEAT EXCHANGER	8,820 SQ FT 16.7 MMBTU/HR	SHELL: 304 SS TUBES: 304 SS	
E-104	PREHEATER	2,260 SQ FT 11.49 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	

Table 6.2 (Continued)
ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONCLUDED)				
E-105	COOLER	2,520 SQ FT 16.3 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-201	COOLER	5,020 SQ FT 18.3 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-202	CONDENSER	4,980 SQ FT 71.6 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-203	REBOILER	9,980 SQ FT 85.4 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-204	CONDENSER	1,720 SQ FT 17.05 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-205	REBOILER	3,400 SQ FT 17.2 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-206	COOLER	60 SQ FT 0.95 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-207	HEAT EXCHANGER	180 SQ FT 0.64 MMBTU/HR	SHELL: 304 SS TUBES: 304 SS	
E-208	COOLER	70 SQ FT 0.63 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-209	EVAPORATOR	730 SQ FT 4.63 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	VERTICAL LONG TUBE EVAPORATOR
E-210	THIN FILM EVAPORATOR	75 SQ FT 0.46 MMBTU/HR	SHELL: 304 SS TUBES: 304 SS	WITH 15 HP DRIVE
E-211	CONDENSER	430 SQ FT 6.66 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-301A,B	COOLER	5,770 SQ FT 32.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-302A,B	HEAT EXCHANGER	10,000 SQ FT 47 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-303A,B	CONDENSER	6,600 SQ FT 38.49 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-304A,B	REBOILER	9,200 SQ FT 130.7 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-305	HEAT EXCHANGER	2,200 SQ FT 7.63 MMBTU/HR	SHELL: C.S. TUBES: C.S.	FOR NOX TREATMENT FACILITIES, NOT SHOWN IN FLOW DIAGRAM
E-306	COOLER	940 SQ FT 0.97 MMBTU/HR	SHELL: C.S. TUBES: C.S.	FOR NOX TREATMENT FACILITIES, NOT SHOWN IN FLOW DIAGRAM
E-401	CONDENSER	6,400 SQ FT 62.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-501	HEATER	300 SQ FT 4.29 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-502	REBOILER	220 SQ FT 1.04 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-503	CONDENSER	1,600 SQ FT 8.2 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-504	CONDENSER	860 SQ FT 13.84 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-505	REBOILER	180 SQ FT 1.1 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-601	COOLER	130 SQ FT 0.34 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	WITH CHILLED WATER COOLING
E-602	CONDENSER	120 SQ FT 0.64 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-603	REBOILER	390 SQ FT 0.96 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	

Table 6.2 (Continued)
ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
ADIPIC ACID
AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
PROCESS FURNACES				
F-301	STARTUP HEATER	8.36 MMBTU/HR	C.S.	USED ONLY FOR START-UP OF NOX TREAT
TANKS				
T-101	CYCLOHEXANE TANK	46,200 GAL	C.S.	
T-102	WASTEWATER TANK	18,700 GAL	C.S.	
T-103	CATALYST DOSING TANK	1,100 GAL	C.S.	
T-151	CYCLOHEXANE STORAGE	550,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-201	EFFLUENT TANK	80,000 GAL	304 SS	
T-202	DILUTE CAUSTIC TANK	16,500 GAL	304 SS	
T-203	HEAVY ENDS RECEIVER	220 GAL	C.S.	
T-204	KA SURGE TANK	44,000 GAL	304 SS	
T-301	RECOVERED ACID TANK	27,500 GAL	316 SS	
T-302	WASTEWATER TANK	74,000 GAL	C.S.	
T-401	SURGE TANK	46,000 GAL	304 SS	
T-402	FILTRATE MIX TANK	62,000 GAL	C.S.	
T-403	ADA SURGE BIN	82,000 GAL	304 SS	
T-451	NITRIC ACID STORAGE	440,000 GAL	316 SS	WITH LOADING FACILITIES
T-452A-D	ADA STORAGE BINS	82,000 GAL	304 SS	NOT SHOWN IN FLOW DIAGRAM
T-501	FRESH NITRIC ACID TANK	37,000 GAL	316 SS	W/ LOADING FACILITIES, NOT SHOWN IN FLOW DIAGRAM
T-502	CATALYST RECYCLE TANK	130 GAL	304 SS	
T-503	MIXED DIBASIC ACIDS TK	72,000 GAL	304 SS	
T-504	DILUTE NITRIC ACID TK	15,000 GAL	316 SS	
T-505	NITRIC ACID TANK	300 GAL	316 SS	
T-601	SULFURIC ACID TANK	35,000 GAL	316 SS	
T-602	WASTE WATER TANK	26,000 GAL	C.S.	
T-603	MONOBASIC ACID TANK	3,000 GAL	304 SS	
T-604	DIBASIC ACID TANK	18,000 GAL	304 SS	
T-651	BY-PRODUCT STORAGE	60,000 GAL	C.S.	
PRESSURE VESSELS				
V-101	SEPARATOR	2,400 GAL	304 SS	
V-102	SEPARATOR	220 GAL	C.S.	
V-201	NEUTRALIZER	5,000 GAL	304 SS CLAD	WITH 30 HP AGITATOR
V-202	SEPARATOR	10,000 GAL	304 SS CLAD	
V-203	NEUTRALIZER	5,000 GAL	304 SS CLAD	WITH 30 HP AGITATOR
V-204	SEPARATOR	5,000 GAL	304 SS CLAD	
V-205	NEUTRALIZER	5,000 GAL	304 SS CLAD	WITH 30 HP AGITATOR
V-206	SEPARATOR	5,000 GAL	304 SS CLAD	
V-207	REFLUX DRUM	1,430 GAL	C.S.	
V-208	REFLUX DRUM	880 GAL	C.S.	
V-209	HYDROLYSIS VESSEL	990 GAL	316 SS	WITH 5 HP AGITATOR
V-301A,B	REFLUX DRUMS	5,000 GAL	C.S.	
V-302	STEAM DRUM	9,500 GAL	C.S.	FOR NOX TREATMENT, NOT SHOWN IN FLOW DIAGRAM
V-401	CONDENSATE RECEIVER	1,650 GAL	316 SS	
V-402	SLURRY VESSEL	1,320 GAL	304 SS	WITH 10 HP AGITATOR
V-403A,B	ADA DISSOLVERS	3,400 GAL	304 SS	WITH 25 HP AGITATOR
V-404	SLURRY VESSEL	1,320 GAL	304 SS	WITH 10 HP AGITATOR
V-501	DISSOLVING VESSEL	1,130 GAL	304 SS	WITH 10 HP AGITATOR
V-502A,B	ION EXCHANGE VESSELS	400 GAL	304 SS	
V-503A,B	ION EXCHANGE VESSELS	400 GAL	304 SS	
V-504	REFLUX DRUM	260 GAL	304 SS	
V-601	ACID DILUTION VESSEL	7,700 GAL	316 SS	
V-602	NEUTRALIZER	2,100 GAL	316 SS	WITH 20 HP AGITATOR
V-603	DECANTER	2,100 GAL	316 SS	
V-604	REFLUX DRUM	500 GAL	316 SS	

Table 6.2 (Concluded)
ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
MISCELLANEOUS EQUIPMENT				
M-101	STATIC MIXER	920 GPM	304 SS	
M-201	STEAM EJECTOR	200 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-301	STATIC MIXER	920 GPM	304 SS	
M-302	STATIC MIXER	920 GPM	304 SS	
M-303	STATIC MIXER	880 GPM	304 SS	
M-304	STEAM EJECTOR	155 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-401	ACTIVE CARBON ABSORBER	1850 GAL	CARBON STEEL	210 CUFT OF ACTIVE CARBON
M-402	ACTIVE CARBON ABSORBER	1850 GAL	CARBON STEEL	210 CUFT OF ACTIVE CARBON
M-403	ACTIVE CARBON ABSORBER	1850 GAL	CARBON STEEL	210 CUFT OF ACTIVE CARBON
M-404	STEAM EJECTOR	20 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-405	SCREW CONVEYOR	17.4 FT, 18 IN DIA.	304 SS	
M-406	ELEVATOR	600 T/D	304 SS	
M-601	STEAM EJECTOR	100 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
SPECIAL EQUIPMENT				
S-401	CRYSTALLIZER	60000 GAL, MULTI-CHA	316 SS	WITH 240 HP AGITATORS
S-402	SEDIMENTATION CENTRIF.	48 IN BOWL DIA.	316 SS	DISK TYPE, WITH 40 HP DRIVE
S-403	CENTRIFUGE	48 IN BOWL DIA.	316 SS	VERTICAL TYPE, AUTOMATIC BATCH CENTRIFUGE
WITH				
S-404	CRYSTALLIZER	36000 GAL, MULTI-CH	316 SS	40 HP DRIVE
S-405	SEDIMENTATION CENTRIF.	40 IN BOWL DIA.	316 SS	DISK TYPE, WITH 35 HP DRIVE
S-406	CENTRIFUGE	40 IN BOWL DIA.	316 SS	VERTICAL TYPE, AUTOMATIC BATCH CENTRIFUGE
WITH				
S-407	ROTARY DRYER	4.5 FT X 25 FT	316 SS	35 HP DRIVE
S-408	ROTARY COOLER	3 FT X 20 FT	316 SS	WITH STEAM TUBES AND 20 HP DRIVE
S-501	CRYSTALLIZER	6000 GAL	316 SS	WITH AIR COOLING AND 20 HP DRIVE
S-502	CENTRIFUGE	24 IN BOWL DIA.	316 SS	VERTICAL TYPE, AUTOMATIC BATCH CENTRIFUGE
WITH				20 HP DRIVE
PUMPS				
SECTION	OPERATING	SPARES	OPERATING BHP	
100	5	5	83	
200	21	21	166	
300	6	6	294	
400	8	8	33	
500	10	10	6	
600	10	1	7	

Table 6.3

ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

TOTAL CAPITAL INVESTMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	3,022	0.59	0.59
COLUMNS	4,774	0.76	0.73
VESSELS & TANKS	4,265	0.59	0.43
HEAT EXCHANGERS	6,663	0.88	0.78
FURNACES	188	0.82	0.82
COMPRESSORS	3,971	0.76	0.76
SPECIAL EQUIPMENT	4,701	0.60	0.60
MISCELLANEOUS EQUIPMENT	599	0.55	0.54
PUMPS	1,538	0.46	0.41

TOTAL	29,721	0.71	0.64
DIRECT INSTALLATION COSTS	56,842	0.48	0.41
INDIRECT COSTS	28,493	0.52	0.43
UNSCHEDULED EQUIPMENT, 10%	11,506	0.55	0.47

BATTERY LIMITS, INSTALLED	126,562	0.55	0.47
CONTINGENCY, 25%	31,640	0.55	0.47

BATTERY LIMITS INVESTMENT	158,202	0.55	0.47
OFF-SITES, INSTALLED			
CLARIFIED WATER	1,253	0.74	0.74
COOLING WATER	6,147	0.92	0.92
PROCESS WATER	737	0.62	0.62
BOILER FEED WATER	2,679	0.54	0.53
STEAM	13,459	0.84	0.81
REFRIGERATION	496	0.71	0.48
INERT GAS	184	0.52	0.52
TANKAGE	4,555	0.58	0.56

UTILITIES & STORAGE	29,511	0.78	0.75
GENERAL SERVICE FACILITIES	37,543	0.59	0.51
WASTE TREATMENT	7,910	0.55	0.47

TOTAL	74,963	0.66	0.60
CONTINGENCY, 25%	18,741	0.66	0.60

OFF-SITES INVESTMENT	93,704	0.66	0.60
TOTAL FIXED CAPITAL	251,906	0.59	0.52

Table 6.4
ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

CAPITAL INVESTMENT BY SECTION

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
ADIPIC ACID
AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	CYCLOHEXANE OXIDATN			KA OIL RECOVERY			KA OXIDATION		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	2,041	0.62	0.62	--	--	--	982	0.52	0.52
COLUMNS	251	0.66	0.66	737	0.67	0.64	3,556	0.80	0.78
VESSELS & TANKS	173	0.67	0.37	1,067	0.66	0.44	484	0.55	0.48
HEAT EXCHANGERS	685	0.85	0.74	1,590	0.81	0.73	3,727	0.92	0.81
FURNACES	--	--	--	--	--	--	188	0.82	0.82
COMPRESSORS	3,805	0.76	0.76	--	--	--	62	0.76	0.76
SPECIAL EQUIPMENT	--	--	--	--	--	--	--	--	--
MISCELLANEOUS EQUIPMENT	11	0.60	0.60	58	0.50	0.50	90	0.54	0.53
PUMPS	142	0.61	0.58	557	0.47	0.42	470	0.54	0.50
TOTAL	7,107	0.72	0.70	4,010	0.70	0.58	9,558	0.80	0.73
DIRECT INSTALLATION COSTS	11,610	0.64	0.54	11,168	0.41	0.39	18,208	0.54	0.44
INDIRECT COSTS	6,161	0.63	0.55	4,996	0.45	0.39	9,140	0.59	0.48
UNSCHEDULED EQUIPMENT, 10%	2,488	0.66	0.59	2,017	0.48	0.42	3,691	0.62	0.52
BATTERY LIMITS INSTALLED	27,367	0.66	0.59	22,190	0.48	0.42	40,597	0.62	0.52
CONTINGENCY, 25%	6,842	0.66	0.59	5,548	0.48	0.42	10,149	0.62	0.52
BATTERY LIMITS INVESTMENT	34,208	0.66	0.59	27,738	0.48	0.42	50,746	0.62	0.52
OFFSITES, INSTALLED									
CLARIFIED WATER	70	0.74	0.74	376	0.74	0.74	512	0.74	0.74
COOLING WATER	300	0.92	0.92	1,956	0.92	0.92	2,438	0.92	0.92
PROCESS WATER	36	0.62	0.62	234	0.62	0.62	292	0.62	0.62
BOILER FEED WATER	696	0.41	0.41	431	0.58	0.58	1,041	0.58	0.58
STEAM	2,874	0.64	0.63	2,843	0.90	0.86	6,721	0.90	0.86
REFRIGERATION	391	0.71	0.48	--	--	--	--	--	--
INERT GAS	85	0.52	0.52	--	--	--	--	--	--
TANKAGE	582	0.65	0.65	--	--	--	--	--	--
UTILITIES & STORAGE	5,034	0.63	0.60	5,841	0.86	0.84	11,004	0.86	0.83

Table 6.4 (Concluded)
ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

CAPITAL INVESTMENT BY SECTION

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
ADIPIC ACID
AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	ADIPIC ACID RECOVERY			RECOVERY OF CATALYST			RECOVERY OF DIACIDS		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	--	--	--	--	--	--	--	--	--
COLUMNS	--	--	--	73	0.37	0.35	156	0.67	0.43
VESSELS & TANKS	980	0.58	0.46	878	0.65	0.43	685	0.38	0.38
HEAT EXCHANGERS	398	0.95	0.82	196	0.83	0.79	67	0.76	0.56
FURNACES	--	--	--	--	--	--	--	--	--
COMPRESSORS	104	0.76	0.76	--	--	--	--	--	--
SPECIAL EQUIPMENT	4,206	0.60	0.60	495	0.60	0.60	--	--	--
MISCELLANEOUS EQUIPMENT	381	0.56	0.56	--	--	--	58	0.50	0.50
PUMPS	182	0.37	0.29	133	0.21	0.19	52	0.19	0.16
TOTAL	6,251	0.62	0.58	1,775	0.62	0.49	1,019	0.45	0.39
DIRECT INSTALLATION COSTS	11,372	0.32	0.32	3,284	0.29	0.25	1,201	0.25	0.21
INDIRECT COSTS	5,801	0.39	0.36	1,665	0.37	0.28	731	0.30	0.24
UNSCHEDULED EQUIPMENT, 10%	2,342	0.42	0.40	672	0.40	0.32	295	0.33	0.27
BATTERY LIMITS INSTALLED	25,766	0.42	0.40	7,396	0.40	0.32	3,246	0.33	0.27
CONTINGENCY, 25%	6,442	0.42	0.40	1,849	0.40	0.32	811	0.33	0.27
BATTERY LIMITS INVESTMENT	32,208	0.42	0.40	9,246	0.40	0.32	4,057	0.33	0.27
OFFSITES, INSTALLED									
CLARIFIED WATER	186	0.74	0.74	105	0.74	0.74	4	0.74	0.74
COOLING WATER	1,062	0.92	0.92	374	0.92	0.92	17	0.92	0.92
PROCESS WATER	127	0.62	0.62	45	0.62	0.62	2	0.62	0.62
BOILER FEED WATER	25	0.58	0.58	464	0.58	0.58	23	0.44	0.44
STEAM	160	0.90	0.86	747	0.90	0.86	113	0.70	0.67
REFRIGERATION	--	--	--	--	--	--	105	0.71	0.48
INERT GAS	--	--	--	99	0.52	0.52	--	--	--
TANKAGE	3,836	0.57	0.56	--	--	--	138	0.65	0.38
UTILITIES & STORAGE	5,396	0.66	0.64	1,834	0.79	0.76	402	0.68	0.51

Table 6.5
ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
CYCLOHEXANE	15.62 ¢/LB	0.73005 LB	11.40
CAUSTIC SODA	11 ¢/LB	0.04991 LB	0.55
COBALT NAPHTHENATE	3.71 \$/LB	0.00075 LB	0.28
NITRIC ACID	18.3 ¢/LB	0.59455 LB	10.88
CUPRIC NITRATE	1.3 \$/LB	0.00014 LB	0.02
AMMONIUM VANADATE	86 ¢/LB	0.00006 LB	0.01
SULFURIC ACID	2.3 ¢/LB	0.08358 LB	0.19
GROSS RAW MATERIALS			23.33
BY-PRODUCTS			
MIXED DIBASIC ACIDS	15 ¢/LB	-0.13546 LB	-2.03
DIBASIC ACIDS	12.9 ¢/LB	-0.13546 LB	-1.75
TOTAL BY-PRODUCTS			-3.78
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	56.8 GAL	474 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	11.3 LB	11.3 KG
STEAM, 600 PSIG	5.72 \$/MLB	1.01 LB	1.01 KG
ELECTRICITY	4 ¢/KWH	0.0508 KWH	0.112 KWH
NATURAL GAS	3.24 \$/MMBTU	1.58 BTU	0.876 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.342 SCF	21.3 LITERS
REFRIGERATION, 40°F	5.09 ¢/TON-HR	0.0035 TON-HR	0.0272 KWH
TOTAL UTILITIES			6.33

Table 6.5 (Concluded)
ADIPIC ACID FROM CYCLOHEXANE BY OXIDATION PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	150	300#	600
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	114.1	158.2	231.4
OFFSITES	62.0	93.7	148.5
TOTAL FIXED CAPITAL (TFC)	176.1	251.9	380.0
SCALING EXPONENTS	0.52	0.59	

PRODUCTION COSTS (\$/LB)

RAW MATERIALS	23.33	23.33	23.33
BY-PRODUCTS	-3.78	-3.78	-3.78
UTILITIES	6.33	6.33	6.33
-----	-----	-----	-----
VARIABLE COSTS	25.88	25.88	25.88
OPERATING LABOR, 12/SHIFT, \$33.58/HR	2.35	1.18	0.59
MAINTENANCE LABOR, 3%/YR OF BLI	2.28	1.58	1.16
CONTROL LAB LABOR, 20% OF OPER LABOR	0.47	0.24	0.12
-----	-----	-----	-----
LABOR COSTS	5.10	3.00	1.87
MAINTENANCE MATERIALS, 3%/YR OF BLI	2.28	1.58	1.16
OPERATING SUPPLIES, 10% OF OPER LABOR	0.23	0.12	0.06
-----	-----	-----	-----
TOTAL DIRECT COSTS	33.49	30.58	28.97
PLANT OVERHEAD, 80% OF LABOR COSTS	4.08	2.40	1.50
TAXES AND INSURANCE, 2%/YR OF TFC	2.35	1.68	1.27
-----	-----	-----	-----
PLANT CASH COSTS	39.92	34.66	31.74
DEPRECIATION, 10%/YR OF TFC	11.74	8.40	6.33
-----	-----	-----	-----
PLANT GATE COSTS	51.66	43.06	38.07
G&A, SALES, RESEARCH	7.00	7.00	7.00
-----	-----	-----	-----
NET PRODUCTION COST	58.66	50.06	45.07
ROI BEFORE TAXES, 25%/YR OF TFC	29.36	20.99	15.83
-----	-----	-----	-----
PRODUCT VALUE	88.02	71.05	60.90

* OF ADIPIC ACID

BASE CASE

ADIPIC ACID FROM BUTADIENE BY THE CARBOHYDROXYLATION PROCESS

Process Description

Figure 6.2 (foldout at end of report) presents the flow diagram for this process, and the utilities summary and major equipment list are given in Table 6.6 and 6.7, respectively. A brief description of the process is given below.

The continuous process described below is SRI's process with design based on current patents assigned to BASF, which are reviewed in PEP report 3B.

Cobalt acetate in aqueous solution is reduced to cobalt carbonyl catalyst and is extracted into C4 fraction feed stream. The resulting mixture is subjected to carbohydroxylation, which takes place in two stages -- first stage at 120°C and 300 atm, and second stage at 130°C and 600 atm. The conversion of butadiene is complete with 91.7% selectivity to methyl pentenoate in the first stage. In the second stage, the conversion of methyl pentenoate is 93% with 78.5% selectivity to dimethyl adipate. After each stage, there is pressure letdown to remove carbon monoxide and other C4's followed by distillation to recover methanol and pyridine. The bottom stream from the distillation in the stage, containing methyl pentenoates, dimethyl adipate and catalyst, passes to catalyst oxidation, where the cobalt catalyst reacts with air to form cobalt acetate. The latter is removed by water extraction and returned to the catalyst reduction operation to form cobalt carbonyl catalyst as mentioned earlier.

The catalyst free stream from the water extraction undergoes distillation in a series of three columns to remove pyridine and monoesters, such as methyl valerate and methyl pentenoate. The former is credited as a by-product, and the latter is recycled to the second stage carbohydroxylation. The crude dimethyl adipate from the bottom of the third column goes to acetal hydrolysis reactor, where a small amount of acetal is converted to light ends that are removed overhead to be sent to incineration. The acetal free crude dimethyl adipate is then distilled to remove heavy ends. The purified dimethyl adipate is hydrolyzed to form adipic acid and methanol. The methanol is distilled and recycled. The adipic acid solution undergoes crystallization, centrifuging, washing, and drying to get final product.

Cost Estimates

Capital investment summary for this process is given in Table 6.8, and those for operation sections are listed in Table 6.9. At a capacity of 300 million lb/yr (136,000 t/yr), the process requires \$179.8 million for the battery limits and \$282.9 million for total fixed capital.

The production costs are summarized in Table 6.10. With a unit price of mixed C4 at 11.74 ¢/lb, the cash cost and the plant gate cost for ADA are estimated at 28.8 ¢/lb and 38.3 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 68.9 ¢/lb.

Table 6.6
ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

UTILITIES SUMMARY

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

UNITS	BATTERY LIMITS		SECTION	SECTION	SECTION	SECTION	SECTION
	TOTAL	100	200	300	400	500	
AVERAGE CONSUMPTIONS							
COOLING WATER	GPM	34,838	--	6,465	7,316	3,401	17,656
ELECTRICITY	KW	5,442	3,953	1,070	39	28	352
INERT GAS, LOW P	M SCF/HR	13	6	7	--	--	--
STEAM, 100 PSIG	M LB/HR	137	--	4	58	5	71
STEAM, 150 PSIG	M LB/HR	108	2	58	4	39	4
STEAM, 200 PSIG	M LB/HR	1	--	1	--	--	--
STEAM, 600 PSIG	M LB/HR	42	--	--	40	2	--
REFRIGERATION, -20°F	TONS	276	--	276	--	--	--
REFRIGERATION, 20°F	TONS	3,182	--	3,182	--	--	--

Table 6.7
ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
ADIPIC ACID
AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101	CATALYST REDUCTION	6.2 FT DIA 93 FT T-T	CLADDING: 304 SS PACKING: ACTIVATED CARBON	74 FT OF PACKING 74 FT OF PACKING
R-201	FIRST STAGE REACTOR	14.3 FT DIA 36 FT T-T	CLADDING: 316 SS TRAYS: 316 SS	3 VALVE TRAYS, 24 INCH SPACING WITH 1510 SQFT COOLING COILS
R-202	SECOND STAGE REACTOR	15.4 FT DIA 39 FT T-T	CLADDING: 316 SS TRAYS: 316 SS	3 VALVE TRAYS, 24 INCH SPACING WITH 1040 COLLING COILS
R-301	CATALYST OXIDATION	4.3 FT DIA 35 FT T-T	CLADDING: 316 SS PACKING: 316 SS	25 FT OF 1 INCH RING PACKING
R-401	ACETAL HYDROLYSIS	6.5 FT DIA 65 FT T-T	CLADDING: 316 SS PACKING: 316 SS	55 FT OF 1 INCH RING PACKING 55 FT OF PACKING
R-501	DIESTER HYDROLYSIS	15 FT DIA 125 FT T-T	CLADDING: 316 SS TRAYS: 316 SS	30 VALVE TRAYS, 36 INCH SPACING
COLUMNS				
C-101	CATALYST EXTRACTOR	5.5 FT DIA 36 FT	SHELL: 316 SS TRAYS: 316 SS	12 VALVE TRAYS, 24 INCH SPACING 12 TRAYS, 24 INCH SPACING AND 50 HP DRIVE
C-201	METHANOL-PYRIDINE COLU	9.5 FT DIA 86 FT	SHELL: 316 SS TRAYS: 316 SS	36 VALVE TRAYS, 24 INCH SPACING
C-202	METHANOL-PYRIDINE COLU	4 FT DIA 40 FT	SHELL: 316 SS TRAYS: 316 SS	20 VALVE TRAYS, 18 INCH SPACING
C-301	DIESTER RECOVERY COLUM	4.5 FT DIA 31 FT	SHELL: 316 SS TRAYS: 316 SS	14 VALVE TRAYS, 18 INCH SPACING
C-302	EXTRACTOR	4.2 FT DIA 45 FT	CLADDING: 316 SS TRAYS: 316 SS	15 SIEVE TRAYS, 24 INCH SPACING
C-303	CATALYST RECOVERY COLU	7.2 FT DIA 70 FT	SHELL: 316 SS TRAYS: 316 SS	15 TRAYS, 24 INCH SPACING AND 30 HP DRIVE
C-304A,B	ION EXCHANGE COLUMNS	2.7 FT DIA 20 FT	CLADDING: 316 SS PACKING: ION EXCHANGER	30 VALVE TRAYS, 24 INCH SPACING
C-305	METHANOL COLUMN	2.7 FT DIA 36 FT	SHELL: 316 SS TRAYS: 316 SS	30 VALVE TRAYS, 12 INCH SPACING
C-401	PYRIDINE RECOVERY	4.2 FT DIA 110 FT	SHELL: 316 SS TRAYS: 316 SS	66 VALVE TRAYS, 18 INCH SPACING
C-402	METHYL VALERATE	2.5 FT DIA 60 FT	SHELL: 316 SS TRAYS: 316 SS	52 VALVE TRAYS, 12 INCH SPACING
C-403	MONOESTER RECOVERY	2 FT DIA 12 FT	SHELL: 316 SS TRAYS: 316 SS	52 VALVE TRAYS, 12 INCH SPACING
C-404	DIMETHYL ADIPATE	8.4 FT DIA 50 FT	SHELL: 316 SS TRAYS: 316 SS	12 VALVE TRAYS, 6 INCH SPACING
				12 VALVE TRAYS, 6 INCH SPACING
				20 VALVE TRAYS, 24 INCH SPACING
				20 VALVE TRAYS, 24 INCH SPACING
COMPRESSORS				
K-101A,B	HYDROGEN COMPRESSOR	170 BHP	C.S.	RECIPROCATING
K-102A,B	CO COMPRESSOR	2,330 BHP	C.S.	
K-103A,B	RECYCLD GAS COMPRESSOR	3 BHP	C.S.	
K-201A,B	CO COMPRESSOR	1,270 BHP	C.S.	FOUR STAGES, THREE INTERCOOLERS
K-202A,B	CO COMPRESSOR	835 BHP	C.S.	FOUR STAGES, THREE INTERCOOLERS
K-501A,B	AIR BLOWER	75 BHP	C.S.	
HEAT EXCHANGERS				
E-101	PREHEATER	190 SQ FT 2.11 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-201	PREHEATER	580 SQ FT 7.97 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-202	CONDENSER	590 SQ FT 2.35 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	

Table 6.7 (Continued)
ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONTINUED)				
E-203	CONDENSER	1,285 SQ FT 3.31 MMBTU/HR	SHELL: 316 SS TUBES: 316 SS	
E-204	EXCHANGER	5,000 SQ FT 4.76 MMBTU/HR	SHELL: 316 SS TUBES: 316 SS	
E-205	CONDENSER	5,290 SQ FT 28.06 MMBTU/HR	SHELL: 316 SS TUBES: 316 SS	
E-206	REBOILER	2,280 SQ FT 30.78 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-207	EXCHANGER	1,750 SQ FT 4.07 MMBTU/HR	SHELL: 316 SS TUBES: 316 SS	
E-208	PREHEATER	180 SQ FT 0.81 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-209	COOLER	1,890 SQ FT 20.47 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-210	CONDENSER	45 SQ FT 0.36 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-211	CONDENSER	1,260 SQ FT 10.12 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-212	REBOILER	820 SQ FT 11.13 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-301	PREHEATER	415 SQ FT 3.19 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-302	EXCHANGER	375 SQ FT 0.32 MMBTU/HR	SHELL: 316 SS TUBES: 316 SS	
E-303	CONDENSER	2,890 SQ FT 26.48 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-304	REBOILER	3,700 SQ FT 29.13 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-305	CONDENSER	3,950 SQ FT 39.65 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-306	REBOILER	4,040 SQ FT 43.61 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-307	CONDENSER	1,380 SQ FT 7.02 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-308	REBOILER	610 SQ FT 7.73 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-401	CONDENSER	350 SQ FT 3.65 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-402	REBOILER	380 SQ FT 4.02 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-403	CONDENSER	150 SQ FT 1.34 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-404	REBOILER	510 SQ FT 1.47 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-405	CONDENSER	430 SQ FT 1.45 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-406	REBOILER	500 SQ FT 1.59 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-407	CONDENSER	30 SQ FT 0.13 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-408	REBOILER	20 SQ FT 0.15 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-409	CONDENSER	2,110 SQ FT 27.44 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-410	INERHEATER	2,300 SQ FT 26.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-501	CONDENSER	5,050 SQ FT 25.63 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	

Table 6.7 (Continued)

ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONCLUDED)				
E-502	REBOILER	4,550 SQ FT 28.2 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-503A,B	CONDENSER	6,060 SQ FT 36.06 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-504	CONDENSER	4,970 SQ FT 114.9 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
TANKS				
T-101	PYRIDINE FEED TANK	20,000 GAL	C.S.	
T-102	METHANOL FEED TANK	123,000 GAL	C.S.	
T-151A-C	MIXED BUTYLENE TANKS	440,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-152	METHANOL STORAGE	613,000 GAL	C.S.	
T-251A,B	MIXED C4S STORAGES	376,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-451	METHYL VALERATE STORAG	43,000 GAL	316 SS	NOT SHOWN IN FLOW DIAGRAM
T-501	SURGE TANK	199,000 GAL	316 SS	
T-502	SURGE TANK	10,000 GAL	304 SS	
T-503	ADIPIC ACID BIN	60,000 GAL	EPOXY LINED	
T-551A-F	ADIPIC ACID STORAGE	120,000 GAL	EPOXY LINED	NOT SHOWN IN FLOW DIAGRAM
T-552	DIABASIC ACIDS STORAGE	168,000 GAL	316 SS	NOT SHOWN IN FLOW DIAGRAM
PRESSURE VESSELS				
V-101	FLASH DRUM	2,300 GAL	316 SS	
V-102	SURGE VESSEL	19,000 GAL	304 SS CLAD	
V-201	FLASH DRUM	6,500 GAL	316 SS CLAD	
V-202	SEPARATOR	5,000 GAL	C.S.	
V-203	FLASH DRUM	6,300 GAL	316 SS CLAD	
V-204	SEPARATOR	1,000 GAL	C.S.	
V-205	SURGE DRUM	5,100 GAL	C.S.	
V-206	REFLUX DRUM	5,600 GAL	304 SS CLAD	
V-207	SURGE DRUM	4,600 GAL	316 SS CLAD	
V-208	FLASH DRUM	5,900 GAL	316 SS CLAD	
V-209	REFLUX DRUM	1,300 GAL	304 SS	
V-301	DECANTER	24,800 GAL	316 SS CLAD	
V-302	REFLUX DRUM	3,100 GAL	316 SS CLAD	
V-303	REFLUX DRUM	4,100 GAL	316 SS CLAD	
V-304A,B	MIXING VESSEL	350 GAL	316 SS	
V-305	REFLUX DRUM	900 GAL	316 SS	
V-401	REFLUX DRUM	900 GAL	316 SS	
V-402	REFLUX DRUM	300 GAL	316 SS	
V-403	REFLUX DRUM	500 GAL	316 SS	
V-404	REFLUX DRUM	100 GAL	316 SS	
V-405	REFLUX DRUM	9,300 GAL	316 SS CLAD	
V-501	REFLUX DRUM	1,600 GAL	316 SS	
V-502	SURGE VESSEL	28,700 GAL	316 SS CLAD	WITH 160 HP AGITATOR
V-503	RECEIVER	14,800 GAL	C.S.	
V-504	RECEIVER	15,400 GAL	C.S.	
MISCELLANEOUS EQUIPMENT				
M-201	VACUUM SYSTEM	50 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-202	VACUUM SYSTEM	50 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-301	WEIGH SCALE	1200 LB DIAL	CARBON STEEL	

Table 6.7 (Concluded)
ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

MAJOR EQUIPMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
MISCELLANEOUS EQUIPMENT (CONCLUDED)				
M-401	VACUUM SYSTEM	50 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-402	VACUUM SYSTEM	14 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-501	VACUUM SYSTEM	90 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-502	VACUUM SYSTEM	250 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
SPECIAL EQUIPMENT				
S-401	THIN FILM EVAPORATOR	110 SQFT	316 SS	WITH 20 HP DRIVE
S-501	FIRST CRYSTALLIZER	600 TONS PER DAY	316 SS	EVAPORATIVE TYPE
S-502	CENTRIFUGE	50 IN BOWL DIA.	316 SS	WITH 120 HP DRIVE
S-503	SECOND CRYSTALLIZER	140 TONS PER DAY	316 SS	EVAPORATIVE TYPE
S-504	SCREW CONVEYOR	450 TONS PER DAY	316 SS	WITH 5 HP DRIVE
S-505	ROTARY DRYER	54 IN DIA, 25 FT LG	304 SS	STEAM TUBE TYPE, WITH 5 PH DRIVE
S-506	CENTRIFUGE	12 IN BOWL DIA	304 SS	SEDIMENTATION TYPE, WITH 20 HP DRIVE
S-507	ROTARY COOLER	36 IN	304 SS	WITH 10 PH DRIVE
S-508	BUCKET ELEVATOR	600 TONS PER DAY	304 SS	WITH 5 HP DRIVE
PUMPS				
SECTION	OPERATING	SPARES	OPERATING BHP	
100	17	10	2,231	
200	13	13	399	
300	10	10	12	
400	11	11	16	
500	9	9	25	

Table 6.8
ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

TOTAL CAPITAL INVESTMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	26,816	0.94	0.93
COLUMNS	1,991	0.58	0.46
VESSELS & TANKS	4,473	0.62	0.60
HEAT EXCHANGERS	5,622	0.85	0.84
COMPRESSORS	9,356	0.76	0.76
SPECIAL EQUIPMENT	3,723	0.57	0.57
MISCELLANEOUS EQUIPMENT	76	0.41	0.40
PUMPS	2,825	0.65	0.61

TOTAL	54,881	0.83	0.80
DIRECT INSTALLATION COSTS	42,153	0.57	0.49
INDIRECT COSTS	33,704	0.68	0.62
UNSCHEDULED EQUIPMENT, 10%	13,074	0.71	0.65

BATTERY LIMITS, INSTALLED	143,811	0.71	0.65
CONTINGENCY, 25%	35,953	0.71	0.65

BATTERY LIMITS INVESTMENT	179,764	0.71	0.65
OFF-SITES, INSTALLED			
CLARIFIED WATER	1,260	0.74	0.74
COOLING WATER	6,730	0.92	0.92
PROCESS WATER	783	0.62	0.62
BOILER FEED WATER	1,804	0.50	0.48
STEAM	9,258	0.85	0.84
REFRIGERATION	8,256	0.70	0.70
INERT GAS	184	0.52	0.52
TANKAGE	3,223	0.65	0.59

UTILITIES & STORAGE	31,498	0.78	0.76
GENERAL SERVICE FACILITIES	42,252	0.72	0.66
WASTE TREATMENT	8,988	0.71	0.65

TOTAL	82,739	0.74	0.70
CONTINGENCY, 25%	20,685	0.74	0.70

OFF-SITES INVESTMENT	103,424	0.74	0.70
TOTAL FIXED CAPITAL	283,188	0.72	0.66

Table 6.9
ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

CAPITAL INVESTMENT BY SECTION

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	CATALYST REDUCTION			CARBONYLATION			CATALYST OXIDATION		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	2,471	0.89	0.89	20,709	0.95	0.95	199	0.82	0.82
COLUMNS	405	0.58	0.55	423	0.82	0.60	554	0.56	0.47
VESSELS & TANKS	363	0.64	0.64	418	0.61	0.54	247	0.59	0.51
HEAT EXCHANGERS	20	0.97	0.71	2,413	0.85	0.85	1,266	0.83	0.85
COMPRESSORS	4,197	0.76	0.76	4,950	0.76	0.76	--	--	--
SPECIAL EQUIPMENT	--	--	--	--	--	--	--	--	--
MISCELLANEOUS EQUIPMENT	--	--	--	22	0.44	0.40	9	0.40	0.40
PUMPS	1,753	0.78	0.73	673	0.48	0.58	132	0.29	0.23
TOTAL	9,210	0.79	0.77	29,609	0.89	0.88	2,408	0.72	0.67
DIRECT INSTALLATION COSTS	10,347	0.77	0.72	14,331	0.61	0.55	5,041	0.38	0.28
INDIRECT COSTS	6,793	0.74	0.71	15,262	0.77	0.73	2,587	0.46	0.36
UNSCHEDULED EQUIPMENT, 10%	2,635	0.77	0.73	5,920	0.80	0.76	1,004	0.49	0.39
BATTERY LIMITS INSTALLED	28,985	0.77	0.73	65,122	0.80	0.76	11,040	0.49	0.39
CONTINGENCY, 25%	7,246	0.77	0.73	16,280	0.80	0.76	2,760	0.49	0.39
BATTERY LIMITS INVESTMENT	36,231	0.77	0.73	81,403	0.80	0.76	13,800	0.49	0.39
OFFSITES, INSTALLED									
CLARIFIED WATER	1	0.74	0.74	358	0.74	0.74	246	0.74	0.74
COOLING WATER	--	--	--	1,948	0.92	0.92	1,233	0.92	0.92
PROCESS WATER	--	--	--	227	0.62	0.62	143	0.62	0.62
BOILER FEED WATER	12	0.58	0.58	323	0.57	0.57	847	0.41	0.40
STEAM	65	0.86	0.95	1,702	0.86	0.94	4,221	0.83	0.73
REFRIGERATION	--	--	--	8,256	0.70	0.70	--	--	--
INERT GAS	85	0.52	0.52	99	0.52	0.52	--	--	--
TANKAGE	2,054	0.65	0.65	878	0.65	0.65	--	--	--
UTILITIES & STORAGE	2,217	0.65	0.65	13,790	0.75	0.75	6,691	0.79	0.71

Table 6.9 (Concluded)
ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

CAPITAL INVESTMENT BY SECTION

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
ADIPIC ACID
AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	DIMETHYL ADIPATE RECOVERY			HYDROLYSIS AND DRYING		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.						
REACTORS	841	0.88	0.95	2,596	0.95	0.85
COLUMNS	608	0.43	0.31	--	--	--
VESSELS & TANKS	118	0.49	0.42	3,326	0.63	0.61
HEAT EXCHANGERS	573	0.84	0.84	1,350	0.85	0.80
COMPRESSORS	--	--	--	209	0.76	0.76
SPECIAL EQUIPMENT	262	0.60	0.60	3,461	0.57	0.57
MISCELLANEOUS EQUIPMENT	10	0.40	0.40	34	0.40	0.40
PUMPS	146	0.28	0.23	121	0.31	0.24
TOTAL	2,557	0.70	0.64	11,097	0.72	0.67
DIRECT INSTALLATION COSTS	4,046	0.28	0.26	8,387	0.45	0.39
INDIRECT COSTS	2,294	0.42	0.36	6,768	0.57	0.51
UNSCHEDULED EQUIPMENT, 10%	890	0.45	0.39	2,625	0.60	0.53
BATTERY LIMITS INSTALLED	9,787	0.45	0.39	28,877	0.60	0.53
CONTINGENCY, 25%	2,447	0.45	0.39	7,219	0.60	0.53
BATTERY LIMITS INVESTMENT	12,234	0.45	0.39	36,096	0.60	0.53
OFFSITES, INSTALLED						
CLARIFIED WATER	114	0.74	0.74	541	0.74	0.74
COOLING WATER	573	0.92	0.92	2,976	0.92	0.92
PROCESS WATER	67	0.62	0.62	346	0.62	0.62
BOILER FEED WATER	245	0.55	0.54	376	0.58	0.58
STEAM	1,282	0.86	0.91	1,988	0.86	0.95
REFRIGERATION	--	--	--	--	--	--
INERT GAS	--	--	--	--	--	--
TANKAGE	291	0.65	0.07	--	--	--
UTILITIES & STORAGE	2,572	0.81	0.74	6,228	0.86	0.87

Table 6.10
ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

PRODUCTION COSTS				
PEP COST INDEX: 624				
VARIABLE COSTS				
	UNIT COST	CONSUMPTION PER LB	¢/LB	
RAW MATERIALS				
HYDROGEN	0.388 ¢/FT^3	0.71231 FT^3	0.28	
CARBON MONOXIDE	0.898 ¢/FT^3	6.31449 FT^3	5.67	
MIXED C4 FEED	11.74 ¢/LB	1.20749 LB	14.18	
METHANOL	6.82 ¢/LB	0.02717 LB	0.19	
PYRIDINE	3.878 \$/LB	0.00326 LB	1.26	
ACETIC ACID	31 ¢/LB	0.0004 LB	0.01	
POTASSIUM SULFATE	100 ¢/LB	0.0002 LB	0.02	
COBALT ACETATE	9.78 \$/LB	0.0003 LB	0.29	
GROSS RAW MATERIALS			21.90	
BY-PRODUCTS				
MIXED C4 BY-PRODUCT	4 ¢/LB	-0.68139 LB	-2.73	
METHYL VALERATE	38 ¢/LB	-0.04533 LB	-1.72	
DIBASIC ACIDS	12.9 ¢/LB	-0.21849 LB	-2.82	
TOTAL BY-PRODUCTS			-7.27	
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG	
UTILITIES				
COOLING WATER	7.45 ¢/MGAL	54.9 GAL	458 LITERS	0.41
STEAM, 150 PSIG	4.51 \$/MLB	6.44 LB	6.44 KG	2.90
STEAM, 600 PSIG	5.72 \$/MLB	1.13 LB	1.13 KG	0.65
ELECTRICITY	4 ¢/KWH	0.143 KWH	0.315 KWH	0.57
INERT GAS, LOW P	0.51 \$/MSCF	0.342 SCF	21.3 LITERS	0.02
REFRIGERATION, -20°F	7.76 ¢/TON-HR	0.00724 TON-HR	0.0561 KWH	0.06
REFRIGERATION, 20°F	5.07 ¢/TON-HR	0.0836 TON-HR	0.648 KWH	0.42
TOTAL UTILITIES			5.03	

Table 6.10 (Concluded)

ADIPIC ACID FROM BUTADIENE BY CARBOALKOXYLATION

PRODUCTION COSTS			
	PEP COST INDEX: 624		
CAPACITY (MILLION LB/YR)*	150	300#	600
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	114.9	179.8	294.0
OFFSITES	63.9	103.4	172.9
TOTAL FIXED CAPITAL (TFC)	178.8	283.2	467.0
SCALING EXPONENTS		0.66	0.72
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	21.90	21.90	21.90
BY-PRODUCTS	-7.27	-7.27	-7.27
UTILITIES	5.03	5.03	5.03
VARIABLE COSTS	19.66	19.66	19.66
OPERATING LABOR, 10/SHIFT, \$33.58/HOUR	1.96	0.98	0.49
MAINTENANCE LABOR, 3%/YR OF BLI	2.30	1.80	1.47
CONTROL LAB LABOR, 20% OF OPER LABOR	0.39	0.20	0.10
LABOR COSTS	4.65	2.98	2.06
MAINTENANCE MATERIALS, 3%/YR OF BLI	2.30	1.80	1.47
OPERATING SUPPLIES, 10% OF OPER LABOR	0.20	0.10	0.05
TOTAL DIRECT COSTS	26.81	24.54	23.24
PLANT OVERHEAD, 80% OF LABOR COSTS	3.72	2.38	1.65
TAXES AND INSURANCE, 2%/YR OF TFC	2.38	1.89	1.56
PLANT CASH COSTS	32.91	28.81	26.45
DEPRECIATION, 10%/YR OF TFC	11.92	9.44	7.78
PLANT GATE COSTS	44.83	38.25	34.23
G&A, SALES, RESEARCH	7.00	7.00	7.00
NET PRODUCTION COST	51.83	45.25	41.23
ROI BEFORE TAXES, 25%/YR OF TFC	29.79	23.60	19.46
PRODUCT VALUE	81.62	68.85	60.69

* OF ADIPIC ACID

BASE CASE

CYCLOHEXANOL FROM BENZENE BY THE PARTIAL HYDROGENATION PROCESS

Process Description

Figure 6.3 (foldout at end of report) presents the flow diagram for this process, and the utilities summary and major equipment list are given in Table 6.11 and 6.12, respectively. A brief description of the process is given below.

The continuous process described below is SRI's process with design based on current patents assigned to Asahi Chemical, which are reviewed in PEP report 3B.

The process begins with partial hydrogenation of benzene in two glass-lined autoclaves in series. The liquid effluent from the bottom of the first reactor passes to the top of the second one. Meanwhile, fresh hydrogen along with a recycled gas is charged parallel to each of the hydrogenators through a sparger near the bottom of each reactor. Excess gas from the reactors is compressed and recycled along with fresh hydrogen. The reaction takes place at 150°C and 51 atm in the presence of Ru/Zn catalyst suspended in an aqueous solution of zinc sulfate with 62% conversion of benzene and 78.7% selectivity to cyclohexene. Cyclohexane is major by-product. The heat of reaction is removed through reflux condenser and cooling jacket. The reactor effluent is cooled and degassed to remove entrained hydrogen, which is recycled after compression. The degassed liquid is centrifuged to remove solid catalyst, and decanted to separate the aqueous solution, part of which is used to reslurry the separated catalyst. The remainder is recycled to the hydrogenator along with the newly formed catalyst slurry. After passing through a drying column, the crude cyclohexene is purified by extractive distillation to remove cyclohexane in the first column, and recover cyclohexene in the second column. The unreacted benzene extracted by adiponitrile is separated from the solvent in a third column, and recycled to the hydrogenation reactors.

Cyclohexene is subjected to hydration in two parallel lines with each line comprising two reactors in series. The hydration takes place at 100°C under autogenous pressure in the presence of ZEM catalyst with 15.8% conversion and 99.9% selectivity to cyclohexanol. The heat of hydration is removed through jacket cooling. The catalyst is recovered from the reactor effluent in same manner as the hydrogenation reaction. The crude cyclohexanol is dried, and is purified by distillation.

Cost Estimates

Capital investment summary for this process is given in Table 6.13, and those for operation sections are listed in Table 6.14. At a capacity of 176 million lb/yr (79,800 t/yr), the process requires \$65.5 million for the battery limits and \$114.4 million for total fixed capital.

The production costs are summarized in Table 6.15. With a unit price of benzene at 9.5 ¢/lb, the cash cost and the plant gate cost for cyclohexanol are estimated at 23.1 ¢/lb and 29.6 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 50.8 ¢/lb.

Table 6.11
CYCLOHEXANOL FROM BENZENE BY
PARTIAL HYDROGENATION AND HYDRATION

UTILITIES SUMMARY

CAPACITY: 176 MILLION LB/YR (79,800 T/YR)
 CYCLOHEXANOL
 AT 0.90 STREAM FACTOR

UNITS	BATTERY LIMITS	SECTION	SECTION
	TOTAL	100	200
AVERAGE CONSUMPTIONS			
COOLING WATER	GPM	11,707	10,256
PROCESS WATER	GPM	10	--
ELECTRICITY	KW	2,331	1,013
INERT GAS, LOW P	M SCF/HR	4	4
STEAM, 100 PSIG	M LB/HR	9	--
STEAM, 150 PSIG	M LB/HR	36	35
STEAM, 200 PSIG	M LB/HR	12	12
STEAM, 600 PSIG	M LB/HR	121	46
REFRIGERATION, 20°F	TONS	1,463	1,463

Table 6.12
CYCLOHEXANOL FROM BENZENE BY
PARTIAL HYDROGENATION AND HYDRATION

MAJOR EQUIPMENT

CAPACITY: 176 MILLION LB/YR (79,800 T/YR)
 CYCLOHEXANOL
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101	FIRST HYDROGENATOR	20,000 GAL	SHELL: GLASS LINED AGITATOR: 304 SS	JACKETED AND EQUIPPED WITH 200 HP TEFL
R-102	SECOND HYDROGENATOR	20,000 GAL	SHELL: GLASS LINED AGITATOR: 304 SS	JACKETED AND EQUIPPED WITH 200 HP TEFL
R-201A,B	FIRST HYDRATORS	20,000 GAL	CLADDING: 316 SS AGITATOR: 316 SS	EACH JACKETED AND EQUIPPED WITH 200 HP TURBINE AGITATOR
R-202A,B	SECOND HYDRATORS	20,000 GAL	CLADDING: 316 SS AGITATOR: 316 SS	EACH JACKETED AND EQUIPPED WITH 200 HP TURBINE AGITATOR
COLUMNS				
C-101A,B	DRYERS	3.7 FT DIA 10 FT	SHELL: C.S. PACKING: 316 SS	9 FT OF 1 INCH RING PACKING
C-102	CYCLOHEXANE COLUMN	8.3 FT DIA 130 FT	SHELL: C.S. TRAYS: C.S.	60 VALVE TRAYS, 24 INCH SPACING 60 TRAYS, 24 INCH SPACING
C-103	CYCLOHEXENE COLUMN	10.2 FT DIA 95 FT	SHELL: C.S. TRAYS: C.S.	42 VALVE TRAYS, 24 INCH SPACING 42 TRAYS, 24 INCH SPACING
C-104	BENZENE COLUMN	16 FT DIA 40 FT	SHELL: C.S. TRAYS: C.S.	9 VALVE TRAYS, 30 INCH SPACING 9 TRAYS, 30 INCH SPACING
C-201A,B	DRYERS	4.2 FT DIA 12 FT	CLADDING: 304 SS PACKING: 316 SS	10 FT OF 1 INCH RING PACKING
C-202	CYCLOHEXANOL COLUMN	9.6 FT DIA 46 FT	CLADDING: 304 SS TRAYS: 316 SS	18 VALVE TRAYS, 24 INCH SPACING 18 VALVE TRAYS, 24 INCH SPACING
C-203	CYCLOHEXENE COLUMN	2 FT DIA 48 FT	CLADDING: 304 SS TRAYS: 316 SS	34 VALVE TRAYS, 12 INCH SPACING 34 VALVE TRAYS, 12 INCH SPACING
COMPRESSORS				
K-101A,B	COMPRESSOR	520 BHP	C.S.	
K-102A,B	COMPRESSOR	4 BHP	C.S.	
K-103A,B	COMPRESSOR	30 BHP	C.S.	
HEAT EXCHANGERS				
E-101	PREHEATER	2,750 SQ FT 28.19 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-102	REFLUX CONDENSER	12 SQ FT 0.03 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-103	REFLUX CONDENSER	12 SQ FT 0.03 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-104	COOLER	2,880 SQ FT 32.11 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-105	CONDENSER	1,540 SQ FT 9.29 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-106	REBOILER	1,312 SQ FT 10.22 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-107	CONDENSER	2,600 SQ FT 16.19 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-108	REBOILER	2,380 SQ FT 17.81 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-109	CONDENSER	1,940 SQ FT 14.29 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	

Table 6.12 (Continued)
CYCLOHEXANOL FROM BENZENE BY
PARTIAL HYDROGENATION AND HYDRATION

MAJOR EQUIPMENT

CAPACITY: 176 MILLION LB/YR (79,800 T/YR)
 CYCLOHEXANOL
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONCLUDED)				
E-110	REBOILER	3,670 SQ FT	SHELL: C.S.	
E-111	HEAT EXCHANGER	15.72 MMBTU/HR 1,350 SQ FT	TUBES: 304 SS SHELL: 304 SS	
E-112	COOLER	3.16 MMBTU/HR 1,480 SQ FT	TUBES: 304 SS SHELL: C.S.	
E-113	AIR HEATER	29.03 MMBTU/HR 1,120 SQ FT	TUBES: 304 SS SHELL: C.S.	FOR REGENERATION OF DRYERS, NOT SHOWN
E-201A,B	PREHEATER	3.16 MMBTU/HR 340 SQ FT	TUBES: 304 SS SHELL: C.S.	
E-202A,B	COOLERS	3.93 MMBTU/HR 680 SQ FT	TUBES: 304 SS SHELL: C.S.	
E-203	EXCHANGER	5.34 MMBTU/HR 520 SQ FT	TUBES: 304 SS SHELL: 304 SS	
E-204	CONDENSER	1.99 MMBTU/HR 5,680 SQ FT	TUBES: 304 SS SHELL: C.S.	
E-205	REBOILER	49.52 MMBTU/HR 3,520 SQ FT	TUBES: 304 SS SHELL: C.S.	
E-206	CONDENSER	54.47 MMBTU/HR 15 SQ FT	TUBES: 304 SS SHELL: C.S.	
E-207	REBOILER	0.1 MMBTU/HR 30 SQ FT	TUBES: C.S. SHELL: C.S.	
E-208	COOLER	0.1 MMBTU/HR 200 SQ FT	TUBES: C.S. SHELL: C.S.	
E-209	COOLER	0.89 MMBTU/HR 400 SQ FT	TUBES: 304 SS SHELL: C.S.	
E-212	REBOILER	1.71 MMBTU/HR 300 SQ FT	TUBES: 316 SS SHELL: C.S.	
		12.51 MMBTU/HR	TUBES: 316 SS	
TANKS				
T-101	BENZENE TANK	100,000 GAL	C.S.	
T-102	SURGE TANK	70,000 GAL	C.S.	
T-103	CYCLOHEXANE TANK	25,600 GAL	C.S.	
T-104	SOLVENT TANK	28,300 GAL	C.S.	
T-151	BENZENE STORAGE	500,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM
T-152	CYCLOHEXANE STORAGE	128,000 GAL	C.S.	
T-201	CYCLOHEXENE TANK	660,000 GAL	304 SS	
T-202	SURGE TANK	270,000 GAL	304 SS	
T-203	CYCLOHEXANOL TANK	35,800 GAL	304 SS	
T-251A,B	CYCLOHEXANOL STORAGE	430,000 GAL	C.S.	NOT SHOWN INFLOW DIAGRAM
PRESSURE VESSELS				
V-101	CATALYST MAKEUP VESSEL	70 GAL	304 SS	
V-102	RESLURRY VESSEL	4,600 GAL	304 SS CLAD	WITH 46 HP AGITATOR
V-103	SEPARATOR	12,000 GAL	304 SS CLAD	
V-104	DECANTER	35,000 GAL	304 SS CLAD	
V-105	REFLUX DRUM	3,200 GAL	C.S.	
V-106	REFLUX DRUM	5,100 GAL	C.S.	
V-107	REFLUX DRUM	2,100 GAL	C.S.	
V-201	CATALYST MAKEUP VESSEL	3,300 GAL	304 SS CLAD	WITH 33 HP AGITATOR
V-202A,B	RESLURRY VESSEL	6,000 GAL	304 SS CLAD	WITH 60 HP AGITATOR
V-203A,B	DECANTERS	34,000 GAL	304 SS CLAD	
V-204	SURGE DRUM	25,000 GAL	C.S.	
V-205	SURGE DRUM	75 GAL	C.S.	

Table 6.12 (Concluded)
CYCLOHEXANOL FROM BENZENE BY
PARTIAL HYDROGENATION AND HYDRATION

MAJOR EQUIPMENT

CAPACITY: 176 MILLION LB/YR (79,800 T/YR)
 CYCLOHEXANOL
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
MISCELLANEOUS EQUIPMENT				
M-101	WEIGH SCALE	50 LB DIAL	CARBON STEEL	
M-102	VACUUM SYSTEM	100 MMHG	CARBON STEEL	
M-103	CARTRIDGE FILTER	70 SQFT	CARBON STEEL	
M-201	WEIGH SCALE	400 LB DIAL	CARBON STEEL	
M-202	CARTRIDGE FILTER	360 SQFT	CARBON STEEL	ROTARY PISTON, SINGLE STAGE, 1.5 HP
SPECIAL EQUIPMENT				
S-101	CENTRIFUGE	25 IN. BOWL DIA.	304 SS	WITH 100 HP HELICAL CONVEYER
S-201A,B	CENTRIFUGE	40 IN. BOWL DIA.	304 SS	EACH EQUIPPED WITH 150 HP HELICAL CONVEYER
PUMPS				
SECTION	OPERATING	SPARES	OPERATING BHP	
100	17	14	130	
200	15	13	338	

Table 6.13
CYCLOHEXANOL FROM BENZENE BY
PARTIAL HYDROGENATION AND HYDRATION

TOTAL CAPITAL INVESTMENT			
CAPACITY: 176 MILLION LB/YR (79,800 T/YR)			
CYCLOHEXANOL			
AT 0.90 STREAM FACTOR			
PEP COST INDEX: 624			
	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	4,634	0.69	0.69
COLUMNS	1,130	0.73	0.52
VESSELS & TANKS	3,507	0.70	0.62
HEAT EXCHANGERS	1,809	0.78	0.76
COMPRESSORS	1,074	0.76	0.76
CENTRIFUGE	807	0.86	0.86
MISCELLANEOUS EQUIPMENT	40	0.53	0.53
PUMPS	507	0.38	0.30

TOTAL	13,507	0.71	0.66
DIRECT INSTALLATION COSTS	21,525	0.41	0.34
INDIRECT COSTS	12,627	0.47	0.40
UNSCHEDULED EQUIPMENT, 10%	4,766	0.52	0.44

BATTERY LIMITS, INSTALLED	52,424	0.52	0.44
CONTINGENCY, 25%	13,106	0.52	0.44

BATTERY LIMITS INVESTMENT	65,530	0.52	0.44
OFF-SITES, INSTALLED			
CLARIFIED WATER	602	0.74	0.70
COOLING WATER	2,499	0.92	0.92
PROCESS WATER	406	0.62	0.62
BOILER FEED WATER	1,656	0.40	0.22
STEAM	8,563	0.91	0.64
REFRIGERATION	3,370	0.70	0.70
INERT GAS	95	0.52	0.27
TANKAGE	1,731	0.65	0.65

UTILITIES & STORAGE	18,922	0.80	0.64
GENERAL SERVICE FACILITIES	16,890	0.59	0.48
WASTE TREATMENT	3,277	0.52	0.44

TOTAL	39,088	0.69	0.55
CONTINGENCY, 25%	9,772	0.69	0.55

OFF-SITES INVESTMENT	48,860	0.69	0.55
TOTAL FIXED CAPITAL	114,391	0.59	0.49

Table 6.14
CYCLOHEXANOL FROM BENZENE BY
PARTIAL HYDROGENATION AND HYDRATION

CAPITAL INVESTMENT BY SECTION

CAPACITY: 176 MILLION LB/YR (79,800 T/YR)
CYCLOHEXANOL
AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

PARTL.HYDROGENATION OF BENZENEHYDRATION OF CYCLOHEXENE

	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.						
REACTORS	2,673	0.70	0.70	1,961	0.67	0.67
COLUMNS	743	0.73	0.51	387	0.74	0.55
VESSELS & TANKS	915	0.70	0.58	2,592	0.70	0.63
HEAT EXCHANGERS	1,236	0.76	0.77	573	0.82	0.74
COMPRESSORS	1,074	0.76	0.76	--	--	--
CENTRIFUGE	192	0.86	0.86	615	0.86	0.86
MISCELLANEOUS EQUIPMENT	11	0.54	0.53	28	0.53	0.53
PUMPS	272	0.37	0.30	235	0.39	0.31
TOTAL	7,117	0.72	0.67	6,390	0.71	0.65
DIRECT INSTALLATION COSTS	11,630	0.45	0.35	9,896	0.36	0.34
INDIRECT COSTS	6,757	0.49	0.40	5,870	0.45	0.39
UNSCHEDULED EQUIPMENT, 10%	2,550	0.54	0.45	2,216	0.49	0.44
BATTERY LIMITS INSTALLED	28,053	0.54	0.45	24,371	0.49	0.44
CONTINGENCY, 25%	7,013	0.54	0.45	6,093	0.49	0.44
BATTERY LIMITS INVESTMENT	35,066	0.54	0.45	30,464	0.49	0.44
OFFSITES, INSTALLED						
CLARIFIED WATER	504	0.74	0.70	98	0.74	0.70
COOLING WATER	2,234	0.92	0.92	265	0.92	0.92
PROCESS WATER	356	0.62	0.62	42	0.62	0.62
BOILER FEED WATER	961	0.32	0.17	695	0.50	0.31
STEAM	4,316	0.89	0.55	4,247	0.94	0.73
REFRIGERATION	3,370	0.70	0.70	--	--	--
INERT GAS	95	0.52	0.27	--	--	--
TANKAGE	773	0.65	0.65	958	0.65	0.65
UTILITIES & STORAGE	12,609	0.78	0.63	6,305	0.85	0.67

Table 6.15
CYCLOHEXANOL FROM BENZENE BY
PARTIAL HYDROGENATION AND HYDRATION

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
HYDROGEN	0.388 ¢/FT^3	10.9707 FT^3	4.26
BENZENE	9.5 ¢/LB	1.09044 LB	10.36
RU/ZN CATALYST	8.66 \$/LB	0.00018 LB	0.16
ZEM CATALYST	2.4 \$/LB	0.00189 LB	0.45
ADIPONITRILE	42 ¢/LB	0.00011 LB	NEGL
GROSS RAW MATERIALS			15.23
BY-PRODUCTS			
CYCLOHEXANE	14.7 ¢/LB	-0.2444 LB	-3.59
TOTAL BY-PRODUCTS			-3.59
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	31.5 GAL	0.23
PROCESS WATER	1.101 \$/MGAL	0.0255 GAL	NEGL
STEAM, 150 PSIG	4.51 \$/MLB	1.99 LB	0.90
STEAM, 600 PSIG	5.72 \$/MLB	5.96 LB	3.41
ELECTRICITY	4 ¢/KWH	0.104 KWH	0.42
INERT GAS, LOW P	0.51 \$/MSCF	0.161 SCF	0.01
REFRIGERATION, 20°F	7.52 ¢/TON-HR	0.0655 TON-HR	0.49
TOTAL UTILITIES			5.46

Table 6.15 (Concluded)
CYCLOHEXANOL FROM BENZENE BY
PARTIAL HYDROGENATION AND HYDRATION

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	88	176#	352
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	48.3	65.5	93.8
OFFSITES	33.3	48.9	78.8
-----	-----	-----	-----
TOTAL FIXED CAPITAL (TFC)	81.5	114.4	172.7
SCALING EXPONENTS	0.49	0.59	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	15.23	15.23	15.23
BY-PRODUCTS	-3.59	-3.59	-3.59
UTILITIES	5.46	5.46	5.46
-----	-----	-----	-----
VARIABLE COSTS	17.10	17.10	17.10
OPERATING LABOR, 4/SHIFT, \$33.58/HOUR	1.34	0.67	0.33
MAINTENANCE LABOR, 3%/YR OF BLI	1.65	1.12	0.80
CONTROL LAB LABOR, 20% OF OPER LABOR	0.27	0.13	0.07
-----	-----	-----	-----
LABOR COSTS	3.26	1.92	1.20
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.65	1.12	0.80
OPERATING SUPPLIES, 10% OF OPER LABOR	0.13	0.07	0.03
-----	-----	-----	-----
TOTAL DIRECT COSTS	22.14	20.21	19.13
PLANT OVERHEAD, 80% OF LABOR COSTS	2.61	1.54	0.96
TAXES AND INSURANCE, 2%/YR OF TFC	1.85	1.30	0.98
-----	-----	-----	-----
PLANT CASH COSTS	26.60	23.05	21.07
DEPRECIATION, 10%/YR OF TFC	9.26	6.50	4.91
-----	-----	-----	-----
PLANT GATE COSTS	35.86	29.55	25.98
G&A, SALES, RESEARCH	5.00	5.00	5.00
-----	-----	-----	-----
NET PRODUCTION COST	40.86	34.55	30.98
ROI BEFORE TAXES, 25%/YR OF TFC	23.16	16.25	12.26
-----	-----	-----	-----
PRODUCT VALUE	64.02	50.80	43.24

* OF CYCLOHEXANOL

BASE CASE

ADIPIC ACID FROM BENZENE BY THE PARTIAL HYDROGENATION PROCESS

This process is an integrated process, which combines the cyclohexanol process presented above with the process which is similar to the oxidation part of the cyclohexane-based adipic acid process presented at the beginning of this section. The process description of this integrated process is thus omitted, and the following presents the economics of this process.

Cost Estimates

Capital investment summary for this process is given in Table 6.16, and those for operation sections are listed in Table 6.17. At a capacity of 300 million lb/yr (136,000 t/yr), the process requires \$166.4 million for the battery limits and \$276.9 million for total fixed capital.

The production costs are summarized in Table 6.18. With a unit price of benzene at 9.5 ¢/lb, the cash cost and the plant gate cost for ADA are estimated at 35.5 ¢/lb and 44.7 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 74.8 ¢/lb.

Table 6.16
**ADIPIC ACID FROM BENZENE VIA CYCLOHEXANOL BY
 PARTIAL HYDROGENATION, HYDRATION AND OXIDATION**

TOTAL CAPITAL INVESTMENT

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	6,336	0.66	0.66
COLUMNS	5,094	0.79	0.72
VESSELS & TANKS	7,172	0.63	0.56
HEAT EXCHANGERS	6,512	0.87	0.79
FURNACES	188	0.82	0.82
COMPRESSORS	1,426	0.76	0.76
CENTRIFUGE	5,667	0.65	0.64
MISCELLANEOUS EQUIPMENT	575	0.55	0.55
PUMPS	1,384	0.42	0.36
-----	-----	-----	-----
TOTAL	34,354	0.71	0.66
DIRECT INSTALLATION COSTS	56,814	0.36	0.32
INDIRECT COSTS	29,851	0.46	0.40
UNSCHEDULED EQUIPMENT, 10%	12,102	0.49	0.43
-----	-----	-----	-----
BATTERY LIMITS, INSTALLED	133,120	0.49	0.43
CONTINGENCY, 25%	33,280	0.49	0.43
-----	-----	-----	-----
BATTERY LIMITS INVESTMENT	166,400	0.49	0.43
OFF-SITES, INSTALLED			
CLARIFIED WATER	1,334	0.74	0.74
COOLING WATER	6,787	0.92	0.92
PROCESS WATER	791	0.62	0.62
BOILER FEED WATER	2,745	0.58	0.58
STEAM	17,420	0.88	0.80
REFRIGERATION	4,968	0.69	0.68
INERT GAS	106	0.52	0.43
TANKAGE	4,859	0.59	0.57
-----	-----	-----	-----
UTILITIES & STORAGE	39,010	0.80	0.75
GENERAL SERVICE FACILITIES	41,082	0.56	0.49
WASTE TREATMENT	8,320	0.49	0.43
-----	-----	-----	-----
TOTAL	88,412	0.66	0.59
CONTINGENCY, 25%	22,103	0.66	0.59
-----	-----	-----	-----
OFF-SITES INVESTMENT	110,515	0.66	0.59
TOTAL FIXED CAPITAL	276,915	0.56	0.49

Table 6.17
**ADIPIC ACID FROM BENZENE VIA CYCLOHEXANOL BY
 PARTIAL HYDROGENATION, HYDRATION AND OXIDATION**

CAPITAL INVESTMENT BY SECTION

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
 ADIPIC ACID
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	PARTL.HYDROGENATION OF BENZENE			HYDRATION OF CYCLOHEXENE			OXIDATION OF CYCLOHEXANOL		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	3,098	0.70	0.70	2,257	0.67	0.67	981	0.52	0.52
COLUMNS	868	0.78	0.63	441	0.80	0.61	3,556	0.80	0.78
VESSELS & TANKS	1,085	0.69	0.66	3,062	0.69	0.67	483	0.55	0.48
HEAT EXCHANGERS	1,452	0.76	0.77	671	0.81	0.75	3,727	0.92	0.81
FURNACES	--	--	--	--	--	--	188	0.82	0.82
COMPRESSORS	1,260	0.76	0.76	--	--	--	62	0.76	0.76
CENTRIFUGE	230	0.86	0.86	737	0.86	0.86	--	--	--
MISCELLANEOUS EQUIPMENT	13	0.55	0.54	32	0.53	0.53	90	0.54	0.53
PUMPS	292	0.39	0.32	253	0.41	0.33	470	0.54	0.50
TOTAL	8,299	0.72	0.69	7,452	0.71	0.68	9,557	0.80	0.73
DIRECT INSTALLATION COSTS	12,959	0.49	0.40	10,578	0.40	0.33	17,546	0.30	0.30
INDIRECT COSTS	6,961	0.55	0.47	5,904	0.50	0.43	8,874	0.46	0.40
UNSCHEDULED EQUIPMENT, 10%	2,822	0.58	0.50	2,393	0.53	0.45	3,598	0.49	0.43
BATTERY LIMITS INSTALLED	31,041	0.58	0.50	26,328	0.53	0.45	39,575	0.49	0.43
CONTINGENCY, 25%	7,760	0.58	0.50	6,582	0.53	0.45	9,894	0.49	0.43
BATTERY LIMITS INVESTMENT	38,801	0.58	0.50	32,910	0.53	0.45	49,469	0.49	0.43
OFFSITES, INSTALLED									
CLARIFIED WATER	484	0.74	0.74	91	0.74	0.74	501	0.74	0.74
COOLING WATER	2,626	0.92	0.92	302	0.92	0.92	2,418	0.92	0.92
PROCESS WATER	304	0.62	0.62	35	0.62	0.62	280	0.62	0.62
BOILER FEED WATER	672	0.58	0.58	679	0.58	0.58	1,224	0.58	0.58
STEAM	4,567	0.92	0.80	4,752	0.94	0.81	7,104	0.82	0.80
REFRIGERATION	4,686	0.70	0.70	--	--	--	--	--	--
INERT GAS	106	0.52	0.43	--	--	--	--	--	--
TANKAGE	886	0.65	0.65	--	--	--	--	--	--
UTILITIES & STORAGE	14,330	0.81	0.76	5,859	0.90	0.78	11,527	0.81	0.79

Table 6.17 (Concluded)
ADIPIC ACID FROM BENZENE VIA CYCLOHEXANOL BY
PARTIAL HYDROGENATION, HYDRATION AND OXIDATION

CAPITAL INVESTMENT BY SECTION

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)
ADIPIC ACID
AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	ADIPIC ACID RECOVERY			RECOVERY OF CATALYST AND			RECOVERY OF DIBASIC ACIDS		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	--	--	--	--	--	--	--	--	--
COLUMNS	--	--	--	73	0.37	0.35	156	0.67	0.43
VESSELS & TANKS	980	0.58	0.46	878	0.65	0.43	684	0.38	0.38
HEAT EXCHANGERS	398	0.95	0.82	196	0.83	0.79	68	0.76	0.56
FURNACES	--	--	--	--	--	--	--	--	--
COMPRESSORS	104	0.76	0.76	--	--	--	--	--	--
CENTRIFUGE	4,206	0.60	0.60	494	0.60	0.60	--	--	--
MISCELLANEOUS EQUIPMENT	381	0.56	0.56	--	--	--	59	0.50	0.50
PUMPS	182	0.37	0.29	134	0.21	0.19	53	0.19	0.16
TOTAL	6,251	0.62	0.58	1,775	0.62	0.49	1,020	0.45	0.39
DIRECT INSTALLATION COSTS	11,368	0.30	0.30	3,230	0.27	0.25	1,132	0.24	0.23
INDIRECT COSTS	5,769	0.38	0.36	1,639	0.36	0.29	704	0.31	0.27
UNSCHEDULED EQUIPMENT, 10%	2,339	0.41	0.38	664	0.39	0.32	286	0.33	0.30
BATTERY LIMITS INSTALLED	25,726	0.41	0.38	7,309	0.39	0.32	3,142	0.33	0.30
CONTINGENCY, 25%	6,432	0.41	0.38	1,827	0.39	0.32	785	0.33	0.30
BATTERY LIMITS INVESTMENT	32,158	0.41	0.38	9,137	0.39	0.32	3,927	0.33	0.30
OFFSITES, INSTALLED									
CLARIFIED WATER	182	0.74	0.74	72	0.74	0.74	4	0.74	0.74
COOLING WATER	1,054	0.92	0.92	371	0.92	0.92	17	0.92	0.92
PROCESS WATER	122	0.62	0.62	43	0.62	0.62	2	0.62	0.62
BOILER FEED WATER	30	0.58	0.58	124	0.58	0.58	15	0.58	0.58
STEAM	177	0.82	0.80	721	0.82	0.80	99	0.90	0.80
REFRIGERATION	--	--	--	--	--	--	282	0.45	0.45
INERT GAS	--	--	--	--	--	--	--	--	--
TANKAGE	3,836	0.57	0.56	--	--	--	138	0.65	0.38
UTILITIES & STORAGE	5,401	0.66	0.64	1,331	0.82	0.80	556	0.61	0.51

Table 6.18
**ADIPIC ACID FROM BENZENE VIA CYCLOHEXANOL BY
 PARTIAL HYDROGENATION, HYDRATION AND OXIDATION**

PRODUCTION COSTS				
PEP COST INDEX: 624				
VARIABLE COSTS				
	UNIT COST	CONSUMPTION PER LB	\$/LB	
RAW MATERIALS				
HYDROGEN	0.388 ¢/FT^3	7.94586 FT^3	3.08	
BENZENE	9.5 ¢/LB	0.78978 LB	7.50	
RUZN CATALYST	8.66 \$/LB	0.00013 LB	0.11	
ZEM CATALYST	2.4 \$/LB	0.00137 LB	0.33	
ADIPONITRILE	42 ¢/LB	0.00008 LB	NEGL	
CUPRIC NITRATE	1.3 \$/LB	0.00014 LB	0.02	
AMMONIUM VANADATE	86 ¢/LB	0.00006 LB	0.01	
NITRIC ACID	18.3 ¢/LB	0.59455 LB	10.88	

GROSS RAW MATERIALS			21.93	
BY-PRODUCTS				
CYCLOHEXANE	14.7 ¢/LB	-0.17702 LB	-2.60	
MIXED DIBASIC ACIDS	12.9 ¢/LB	-0.05837 LB	-0.75	

TOTAL BY-PRODUCTS			-3.35	
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG	
UTILITIES				
COOLING WATER	7.45 ¢/MGAL	58.9 GAL	491 LITERS	0.44
PROCESS WATER	1.101 \$/MGAL	0.0185 GAL	0.154 LITERS	NEGL
STEAM, 150 PSIG	4.51 \$/MLB	10.3 LB	10.3 KG	4.65
STEAM, 600 PSIG	5.72 \$/MLB	4.15 LB	4.15 KG	2.38
ELECTRICITY	4 ¢/KWH	0.0929 KWH	0.205 KWH	0.37
NATURAL GAS	3.24 \$/MMBTU	10.8 BTU	5.99 KCAL	NEGL
INERT GAS, LOW P	0.51 \$/MSCF	0.116 SCF	7.27 LITERS	0.01
REFRIGERATION, 20°F	7.53 ¢/TON-HR	0.0475 TON-HR	0.368 KWH	0.36
REFRIGERATION, 40°F	5.42 ¢/TON-HR	0.000746 TON-HR	0.00579 KWH	NEGL

TOTAL UTILITIES			8.21	

Table 6.18 (Concluded)
ADIPIC ACID FROM BENZENE VIA CYCLOHEXANOL BY
PARTIAL HYDROGENATION, HYDRATION AND OXIDATION

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	150	300#	600
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	123.4	166.4	234.2
OFFSITES	73.3	110.5	175.1
TOTAL FIXED CAPITAL (TFC)	196.7	276.9	409.3
SCALING EXPONENTS		0.49	0.56
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	21.93	21.93	21.93
BY-PRODUCTS	-3.35	-3.35	-3.35
UTILITIES	8.21	8.21	8.21
VARIABLE COSTS	26.79	26.79	26.79
OPERATING LABOR, 10/SHIFT, \$33.58/HOUR	1.96	0.98	0.49
MAINTENANCE LABOR, 3%/YR OF BLI	2.47	1.66	1.17
CONTROL LAB LABOR, 20% OF OPER LABOR	0.39	0.20	0.10
LABOR COSTS	4.82	2.84	1.76
MAINTENANCE MATERIALS, 3%/YR OF BLI	2.47	1.66	1.17
OPERATING SUPPLIES, 10% OF OPER LABOR	0.20	0.10	0.05
TOTAL DIRECT COSTS	34.28	31.39	29.77
PLANT OVERHEAD, 80% OF LABOR COSTS	3.86	2.27	1.41
TAXES AND INSURANCE, 2%/YR OF TFC	2.62	1.85	1.36
PLANT CASH COSTS	40.76	35.51	32.54
DEPRECIATION, 10%/YR OF TFC	13.11	9.23	6.82
PLANT GATE COSTS	53.87	44.74	39.36
G&A, SALES, RESEARCH	7.00	7.00	7.00
NET PRODUCTION COST	60.87	51.74	46.36
ROI BEFORE TAXES, 25%/YR OF TFC	32.79	23.08	17.05
PRODUCT VALUE	93.66	74.82	63.41

* OF ADIPIC ACID

BASE CASE

COMMERCIAL PROCESSES FOR HMDA

Commercially, HMDA is produced by hydrogenation of adiponitrile, which is mostly prepared from butadiene by hydrocyanation process, and is also produced, to a less extent, by electrohydrodimerization process. For many years, HMDA was also produced from adipic acid by reacting with ammonia over a dehydration catalyst. This process is no longer used in the major producing regions in the world. In the 1970s, Celanese Chemical produced HMDA from cyclohexane via 1,6-hexanediol; this process was dismantled after the company withdrew from the nylon 66 and its intermediates business.

In this report, we present the economics for the production of HMDA by hydrogenation of ADN, and for the coproduction of HMDA and CAPM by partial hydrogenation.

HMDA FROM BUTADIENE BY THE HYDROCYANATION PROCESS

Process Description

Figure 6.4 (foldout at end of report) presents the flow diagram for the butadiene-based HMDA process, and the utilities summary and major equipment list are given in Table 6.19 and 6.20, respectively. The following is a brief description of the process.

The continuous HMDA process described below is SRI's process design based on patents issued to DuPont.

In this process, liquid butadiene is subjected to two-stage hydrocyanation in two cascaded reactors in the first stage to produce pentenenitriles at 110°C and 15 kg/cm². In the second stage, three cascaded reactors are used, wherein the pentenenitriles are further hydrocyanated to adiponitrile at 50°C and 8 kg/cm². Some small amounts of 2-methyl-3-butenenitrile are converted to pentenenitrile in an isomerization reactor between the two stages of hydrocyanation. The hydrocyanation takes place in the presence of a pentenenitrile solution containing tri-o-tolylphosphite and its complex with Ni(0). The same catalyst is also used in the isomerization reaction. The spent nickel catalyst is regenerated by treatment of ammonia.

The adiponitrile from the hydrocyanation reaction is hydrogenated continuously in a fixed-bed reactor packed with reduced iron oxide catalyst. The reaction takes place in excess ammonia at 138°C and 310 kg/cm². After separation of excess ammonia, the crude HMDA is first stripped to remove by-product, hexamethyleneimine. It is then subjected to vacuum distillation in a series of three columns to obtain purified HMDA.

Product overall yield, based on butadiene, is 85.9%. HMDA is primarily used as one of the two monomers for the production of nylon 6,6 fibers and resins.

Cost Estimates

Capital investment summary for this process is given in Table 6.21, and those for operation sections are listed in Table 6.22. At a capacity of 200 million lb/yr (90,700 t/yr), the process requires \$95 million for the battery limits and \$156.3 million for total fixed capital.

The production costs are summarized in Table 6.23. With a unit price of butadiene at 13 ¢/lb, the cash cost and the plant gate cost for HMDA are estimated at 57.2 ¢/lb and 65 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for CAPM is estimated at 93.5 ¢/lb.

Table 6.19
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

UTILITIES SUMMARY

CAPACITY: 200 MILLION LB/YR (90,700 T/YR)
 HMDA
 AT 0.90 STREAM FACTOR

UNITS	BATTERY LIMITS		SECTION	SECTION	SECTION	SECTION	SECTION	SECTION
	TOTAL	100	200	300	400	500	600	
AVERAGE CONSUMPTIONS								
COOLING WATER	GPM	19,621	2,397	224	2,693	2,497	108	11,702
PROCESS WATER	GPM	62	--	--	62	--	--	0
ELECTRICITY	KW	3,820	211	104	586	2	41	2,875
NATURAL GAS	MM BTU/HR	2	--	--	--	--	2	--
INERT GAS, LOW P	M SCF/HR	5	1	0	1	1	--	2
STEAM, 100 PSIG	M LB/HR	26	4	0	18	--	0	3
STEAM, 150 PSIG	M LB/HR	30	13	3	7	1	--	5
STEAM, 250 PSIG	M LB/HR	10	--	--	10	--	--	--
STEAM, 350 PSIG	M LB/HR	17	--	--	--	17	--	--
STEAM, 500 PSIG	M LB/HR	132	--	--	--	18	--	113
REFRIGERATION, 40°F	TONS	536	--	--	517	--	19	--

Table 6.20
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

MAJOR EQUIPMENT

CAPACITY: 200 MILLION LB/YR (90,700 T/YR)
 HMDA
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101	HYDROCYANATION REACTOR	11,000 GAL	CLADDING: 316 SS AGITATOR: 316 SS	WITH 100 HP TURBINE AGITATOR AND 100 SQFT COOLING COILS
R-102	HYDROCYANATION REACTOR	11,000 GAL	CLADDING: 316 SS AGITATOR: 316 SS	WITH 100 HP TURBINE AGITATOR
R-201	ISOMERIZATION REACTOR	14,000 GAL	CLADDING: 316 SS AGITATOR: 316 SS	WITH 120 HP TURBINE AGITATOR
R-301	HYDROCYANATION REACTOR	20,000 GAL	CLADDING: 316 SS AGITATOR: 316 SS	WITH 160 HP AGITATOR AND 1320 SQFT COOLING COILS
R-302	HYDROCYANATION REACTOR	20,000 GAL	CLADDING: 316 SS AGITATOR: 316 SS	WITH 160 HP AGITATOR AND 790 SQFT COOLING COILS
R-303	HYDROCYANATION REACTOR	20,000 GAL	CLADDING: 316 SS AGITATOR: 316 SS	WITH 160 HP AGITATOR AND 790 SQFT COOLING COILS
R-501	CATALYST REACTOR	2,500 GAL	CLADDING: 316 SS AGITATOR: 316 SS	WITH 10 HP AGITATOR.
R-601	HYDROGENATOR	6 FT DIA 36 FT T-T	CLADDING: 316 SS PACKING: SILICA GEL	30 FT OF PACKING
COLUMNS				
C-101	METHYL BUTENENITRILE C	14 FT DIA 76 FT	CLADDING: 316 SS TRAYS: 316 SS	32 SIEVE TRAYS, 24 INCH SPACING
C-201	PN RECOVERY COLUMN	6 FT DIA 84 FT	CLADDING: 316 SS TRAYS: 316 SS	36 SIEVE TRAYS, 24 INCH SPACING
C-301	EXTRACTOR	6 FT DIA 36 FT	CLADDING: 316 SS TRAYS: 316 SS	16 VALVE TRAYS, 18 INCH SPACING ROTATING DISK WITH 5 HP DRIVE
C-302	CYCLOHEXANE COLUMN	3.7 FT DIA 39 FT	CLADDING: 316 SS TRAYS: 316 SS	18 SIEVE TRAYS, 18 INCH SPACING
C-303	CRUDE ADN COLUMN	5 FT DIA 23 FT	CLADDING: 316 SS TRAYS: 316 SS	7 SIEVE TRAYS, 18 INCH SPACING
C-401	ISOMER COLUMN	16 FT DIA 44 FT	CLADDING: 316 SS PACKING: PORCELAIN	36 FT OF 2 INCH RING PACKING
C-402	ADN PURIFICATION COLMN	16 FT DIA 44 FT	CLADDING: 316 SS PACKING: PORCELAIN	36 FT OF 2 INCH RING PACKING
C-501	NITRIC OXIDE SCRUBBER	2 FT DIA 20 FT	CLADDING: 316 SS PACKING: PORCELAIN	15 FT OF 1 INCH RING PACKING
C-601	IMINE STRIPPER	2 FT DIA 25 FT	CLADDING: 316 SS PACKING: PORCELAIN	15 FT OF 1.5 INCH RING PACKING
C-602	CONCENTRATOR	3.2 FT DIA 56 FT	CLADDING: 316 SS TRAYS: 316 SS	50 SIEVE TRAYS, 12 INCH SPACING
C-603	MEDIUM BOILER STRIPPER	2.8 FT DIA 56 FT	CLADDING: 316 SS TRAYS: 316 SS	50 SIEVE TRAYS, 12 INCH SPACING
C-604	HMDA COULMN	12 FT DIA 90 FT	CLADDING: 316 SS TRAYS: 316 SS	40 SIEVE TRAYS, 24 INCH SPACING
COMPRESSORS				
K-601A,B	HYDROGEN COMPRESSOR	1,200 BHP	C.S.	2 STAGES WITH AN INTERCOOLER, ONE SPARE
K-602A,B	HYDROGEN COMPRESSOR	120 BHP	C.S.	ONE SPARE
K-603A,B	HYDROGEN COMPRESSOR	1,600 BHP	C.S.	2 STAGES WITH AN INTERCOOLER, ONE SPARE
K-604A,B	AMMONIA COMPRESSOR	180 BHP	C.S.	TWO STAGES WITH INTERCOOLER, ONE SPARE

Table 6.20 (Continued)
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

MAJOR EQUIPMENT

CAPACITY: 200 MILLION LB/YR (90,700 T/YR)
 HMDA
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS				
E-101	PREHEATER	140 SQ FT 2.53 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-102	EVAPORATOR	210 SQ FT 3.3 MMBTU/HR	SHELL: 316 SS TUBES: 316 SS	
E-103	CONDENSER	890 SQ FT 3.61 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-104	CONDENSER	2,160 SQ FT 8.51 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-105	REBOILER	580 SQ FT 8.94 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-201	CONDENSER	500 SQ FT 2.12 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-202	CONDENSER	30 SQ FT 0.12 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-203	REBOILER	180 SQ FT 2.36 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-301	EVAPORATOR	860 SQ FT 7.04 MMBTU/HR	SHELL: 316 SS TUBES: 316 SS	
E-302	COOLER	410 SQ FT 2.71 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-303	COOLER	400 SQ FT 1.7 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-304	EVAPORATOR	600 SQ FT 8.91 MMBTU/HR	SHELL: 316 SS TUBES: 316 SS	
E-305	CONDENSER	1,270 SQ FT 7.74 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-306	CONDENSER	670 SQ FT 4.5 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-307	REBOILER	330 SQ FT 4.95 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-308	CONDENSER	1,280 SQ FT 3.6 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-309	REBOILER	740 SQ FT 3.96 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-310	CONDENSER	10 SQ FT 0.01 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-401	CONDENSER	1,100 SQ FT 12.42 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-402	REBOILER	3,140 SQ FT 13.67 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-403	CONDENSER	770 SQ FT 12.55 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-404	REBOILER	1,970 SQ FT 13.8 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-501	EVAPORATOR	20 SQ FT 0.22 MMBTU/HR	SHELL: 316 SS TUBES: 316 SS	
E-502	CONDENSER	30 SQ FT 0.23 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-503	COOLER	330 SQ FT 1.08 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-601	PREHEATER	100 SQ FT 1.27 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-602A,B	EVAPORATOR	7,930 SQ FT 76.24 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-603	PARTIAL CONDENSER	3,540 SQ FT 78.71 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	

Table 6.20 (Continued)
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

MAJOR EQUIPMENT

CAPACITY: 200 MILLION LB/YR (90,700 T/YR)
 HMDA
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
HEAT EXCHANGERS (CONCLUDED)				
E-604	PARTIAL CONDENSER	1,380 SQ FT 25.2 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-605	PARTIAL CONDENSER	100 SQ FT 1.03 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-606	CONDENSER	150 SQ FT 1.13 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-607	REBOILER	140 SQ FT 2.1 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-608	CONDENSER	130 SQ FT 1.4 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-609	REBOILER	260 SQ FT 1.47 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-610	CONDENSER	25 SQ FT 0.23 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-611	REBOILER	20 SQ FT 0.25 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-612	CONDENSER	2,640 SQ FT 9.32 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
E-613	REBOILER	2,600 SQ FT 8.93 MMBTU/HR	SHELL: C.S. TUBES: 316 SS	
TANKS				
T-101	TTP LIGAND TANK	1,200 GAL	316 SS	
T-102	MIXING TANK	7,500 GAL	316 SS	
T-151	BUTADIENE STORAGE	320,000 GAL	C.S.	NOT SHOWN IN FLOW DIAGRAM.
T-152A-D	HCN STORAGE	75,000 GAL	304 SS	NOT SHOWN IN FLOW DIAGRAM.
T-201	SURGE TANK	3,200 GAL	316 SS	
T-301	MIXING TANK	45,000 GAL	316 SS	WITH 150 HP AGITATOR.
T-302	FEED TANK	12,000 GAL	316 SS	
T-303	WASTE WATER TANK	42,000 GAL	C.S.	
T-401A,B	ADIPONITRILE TANK	40,000 GAL	304 SS	
T-601	HEXAMETHYLENE IMINE TK	5,000 GAL	304 SS	
T-602	SURGE TANK	90,000 GAL	316 SS	
T-603	HMDA TANK	36,000 GAL	316 SS	
T-651	HMDA LOADING TANK	86,000 GAL	316 SS	NOT SHOWN IN FLOW DIAGRAM
PRESSURE VESSELS				
V-101	BUTADIENE FEED VESSEL	5,500 GAL	C.S.	
V-102	HCN FEED VESSEL	5,000 GAL	304 SS CLAD	
V-103	REFLUX DRUM	2,200 GAL	316 SS CLAD	
V-104	REFLUX DRUM	1,000 GAL	316 SS CLAD	
V-201	REFLUX DRUM	250 GAL	316 SS	
V-202	PN AND ISOMERS SURGE	120 GAL	316 SS	
V-301	CYCLOHEXANE SURGE VESL	4,000 GAL	C.S.	
V-302	DECANTER	7,700 GAL	316 SS	
V-303	SURGE VESSEL	6,400 GAL	316 SS	
V-304	DECANTER	3,800 GAL	316 SS	
V-305	REFLUX DRUM	900 GAL	316 SS	
V-306	MIXING VESSEL	850 GAL	316 SS	WITH 3 HP AGITATOR
V-307	SULFITE MIXING VESSEL	8,000 GAL	304 SS CLAD	WITH 25 HP AGITATOR.
V-308	PN RECOVERY VESSEL	900 GAL	316 SS CLAD	WITH 3 HP AGITATOR
V-309	DECANTER	3,000 GAL	316 SS CLAD	
V-310	REFLUX DRUM	700 GAL	316 SS	

Table 6.20 (Concluded)
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

MAJOR EQUIPMENT

CAPACITY: 200 MILLION LB/YR (90,700 T/YR)
 HMDA
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
PRESSURE VESSELS (CONCLUDED)				
V-311	SURGE VESSEL	7,000 GAL	316 SS CLAD	
V-401	REFLUX DRUM	50 GAL	316 SS	
V-402	REFLUX DRUM	550 GAL	316 SS	
V-501	AMMONIA WATER VESSEL	400 GAL	C.S.	
V-502	TRIPHENYLBORANE VESSEL	500 GAL	316 SS	WITH 2 HP AGITATOR
V-503	TPB SOLUTION VESSEL	750 GAL	316 SS	WITH 5 HP AGITATOR
V-601	SEPARATOR	10,600 GAL	316 SS CLAD	
V-602	SEPARATOR	5,900 GAL	316 SS CLAD	
V-603	SEPARATOR	4,700 GAL	316 SS CLAD	
V-604	REFLUX DRUM	120 GAL	316 SS	
V-605	RECEIVER	120 GAL	304 SS	
V-606	REFLUX DRUM	500 GAL	316 SS	
V-607	REFLUX DRUM	100 GAL	C.S.	
V-608	REFLUX DRUM	30,000 GAL	316 SS CLAD	
MISCELLANEOUS EQUIPMENT				
M-101	VACUUM SYSTEM	40 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-201	VACUUM SYSTEM	40 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM
M-301	CONVEYOR	6 X 30 FT	304 SS	WITH 1.5 HP DRIVE
M-302	CONVEYOR	6 X 30 FT	304 SS	WITH 1.5 HP DRIVE
M-303	CONVEYOR	6 X 30 FT	304 SS	WITH 1.5 HP DRIVE
M-304	VACUUM SYSTEM	200 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAN
M-305	VACUUM SYSTEM	20 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAN
M-401	VACCUM SYSTEM	27 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAN
M-402	VACUUM SYSTEM	27 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAN
M-501	CONVEYOR	6 X 30 FT	304 SS	WITH 1.5 HP DRIVE
M-502	AIR BLOWER	50 INCHES DIA.	304 SS	CENTRIFUGAL, 7 HP
M-503	CONVEYOR	6 X 30 FT	304 SS	WITH 1.5 HP DRIVE
M-601	VACUUM SYSTEM	150 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAN
M-602	VACUUM SYSTEM	20 MMHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAN
SPECIAL EQUIPMENT				
S-101	CENTRIFUGE	24 IN BOWL DIAMETER	316 SS	DISK TYPE WITH 7.5 HP.
S-201	CENTRIFUGE	14 IN BOWL DIAMETER	316 SS	DISK TYPE WITH 6 HP.
S-301	CENTRIFUGE	24 IN BOWL DIAMETER	316 SS	DISK TYPE WITH 7.5 HP.
S-302	CENTRIFUGE	14 IN BOWL DIAMETER	316 SS	DISK TYPE WITH 6 HP.
S-303	DRYER	2 FT DIA., 15 FT LG.	316 SS	WITH 6 HP.
S-501	CENTRIFUGE	7 IN BOWL DIAMETER	316 SS	DISK TYPE WITH 3 HP.
S-502	CENTRIFUGE	7 IN BOWL DIAMETER	316 SS	DISK TYPE WITH 3 HP.
S-503	KILN	5.5 FT DIA., 100 FT	316 SS	ROTARY TYPE WITH 20 HP DRIVE
S-504	COMBUSTION CHAMBER	3 FT X 25 LG.	CARBON STEEL	4 IN BRICK LINING, 1 IN MOTAR BACKING
S-601	CARBON DIOXIDE UNIT	42 LB/HR	CARBON STEEL	12 TON STORAGE TANK AND A VAPORIZER
PUMPS				
SECTION	OPERATING	SPARES	OPERATING BHP	
100	10	9	17	
200	7	7	2	
300	24	23	24	
400	6	5	3	
500	6	6	1	
600	13	13	378	

Table 6.21
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

TOTAL CAPITAL INVESTMENT

CAPACITY: 200 MILLION LB/YR (90,700 T/YR)
 HMDA
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	4,030	0.87	0.78
COLUMNS	2,570	0.85	0.62
VESSELS & TANKS	4,486	0.74	0.57
HEAT EXCHANGERS	3,655	0.85	0.80
COMPRESSORS	4,564	0.76	0.76
SPECIAL EQUIPMENT	831	0.60	0.60
MISCELLANEOUS EQUIPMENT	324	0.58	0.58
PUMPS	927	0.29	0.27

TOTAL	21,388	0.78	0.68
DIRECT INSTALLATION COSTS	29,694	0.50	0.37
INDIRECT COSTS	18,016	0.57	0.45
UNSCHEDULED EQUIPMENT, 10%	6,910	0.61	0.48

BATTERY LIMITS, INSTALLED	76,007	0.61	0.48
CONTINGENCY, 25%	19,002	0.61	0.48

BATTERY LIMITS INVESTMENT	95,009	0.61	0.48
OFF-SITES, INSTALLED			
CLARIFIED WATER	795	0.74	0.74
COOLING WATER	3,603	0.92	0.92
PROCESS WATER	520	0.62	0.62
BOILER FEED WATER	1,765	0.47	0.32
STEAM	9,924	0.91	0.70
REFRIGERATION	1,323	0.95	0.71
INERT GAS	112	0.52	0.52
TANKAGE	2,995	0.83	0.76

UTILITIES & STORAGE	21,039	0.86	0.71
GENERAL SERVICE FACILITIES	23,210	0.66	0.52
WASTE TREATMENT	4,750	0.61	0.48

TOTAL	48,999	0.74	0.59
CONTINGENCY, 25%	12,250	0.74	0.59

OFF-SITES INVESTMENT	61,248	0.74	0.59
TOTAL FIXED CAPITAL	156,257	0.66	0.53

Table 6.22
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

CAPITAL INVESTMENT BY SECTION

CAPACITY: 200 MILLION LB/YR (90,700 T/YR)

HMDA

AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	HYDROCYANATION OF BUTADIENE			ISOMERIZATION OF PENTENENITRILES			HYDROCYANATION OF 3-PENTENENITRILE		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	811	0.75	0.75	391	0.73	0.73	1,822	0.71	0.71
COLUMNS	543	0.95	0.65	174	0.59	0.34	214	0.52	0.44
VESSELS & TANKS	368	0.56	0.44	126	0.35	0.34	1,042	0.66	0.43
HEAT EXCHANGERS	347	0.85	0.84	83	0.85	0.78	591	0.84	0.84
COMPRESSORS	--	--	--	--	--	--	--	--	--
SPECIAL EQUIPMENT	138	0.60	0.60	62	0.60	0.60	294	0.60	0.60
MISCELLANEOUS EQUIPMENT	12	0.56	0.56	12	0.56	0.56	60	0.56	0.56
PUMPS	113	0.24	0.19	61	0.11	0.08	268	0.21	0.17
TOTAL	2,332	0.76	0.64	910	0.62	0.53	4,292	0.67	0.59
DIRECT INSTALLATION COSTS	4,085	0.31	0.30	2,042	0.36	0.30	8,092	0.31	0.26
INDIRECT COSTS	2,263	0.43	0.37	1,041	0.39	0.33	4,368	0.39	0.32
UNSCHEDULED EQUIPMENT, 10%	868	0.47	0.41	399	0.43	0.36	1,675	0.43	0.35
BATTERY LIMITS INSTALLED	9,549	0.47	0.41	4,393	0.43	0.36	18,427	0.43	0.35
CONTINGENCY, 25%	2,387	0.47	0.41	1,098	0.43	0.36	4,607	0.43	0.35
BATTERY LIMITS INVESTMENT	11,936	0.47	0.41	5,492	0.43	0.36	23,034	0.43	0.35
OFFSITES, INSTALLED									
CLARIFIED WATER	89	0.74	0.74	9	0.74	0.74	144	0.74	0.74
COOLING WATER	425	0.92	0.92	40	0.92	0.92	597	0.92	0.92
PROCESS WATER	60	0.62	0.62	6	0.62	0.62	84	0.62	0.62
BOILER FEED WATER	208	0.24	0.00	42	0.24	0.00	362	0.31	0.09
STEAM	592	0.74	0.31	119	0.74	0.31	1,333	0.82	0.48
REFRIGERATION	--	--	--	--	--	--	1,275	0.95	0.71
INERT GAS	22	0.52	0.52	11	0.52	0.52	22	0.52	0.52
TANKAGE	2,539	0.86	0.78	--	--	--	--	--	--
UTILITIES & STORAGE	3,935	0.81	0.66	226	0.68	0.37	3,818	0.83	0.58

Table 6.22 (Concluded)
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

CAPITAL INVESTMENT BY SECTION

CAPACITY: 200 MILLION LB/YR (90,700 T/YR)

HMDA

AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

	PURIFICATION OF ADIPONITRILE			CATALYST PREPARATION			HYDROGENATION OF ADIPONITRILE		
	COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT		COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	--	--	--	106	0.68	0.59	900	1.28	1.03
COLUMNS	924	0.95	0.72	25	0.45	0.69	690	0.80	0.60
VESSELS & TANKS	414	0.68	0.35	74	0.40	0.36	2,461	0.83	0.72
HEAT EXCHANGERS	647	0.81	0.83	51	0.66	0.59	1,936	0.88	0.78
COMPRESSORS	--	--	--	--	--	--	4,564	0.76	0.76
SPECIAL EQUIPMENT	--	--	--	295	0.60	0.60	43	0.60	0.60
MISCELLANEOUS EQUIPMENT	24	0.56	0.56	149	0.59	0.59	67	0.56	0.56
PUMPS	55	0.16	0.13	51	0.18	0.18	379	0.41	0.45
TOTAL	2,064	0.83	0.65	752	0.57	0.54	11,038	0.84	0.75
DIRECT INSTALLATION COSTS	1,712	0.76	0.24	1,580	0.25	0.19	12,181	0.68	0.55
INDIRECT COSTS	1,332	0.75	0.41	822	0.31	0.25	8,189	0.70	0.60
UNSCHEDEDULED EQUIPMENT, 10%	511	0.79	0.44	315	0.35	0.28	3,141	0.74	0.63
BATTERY LIMITS INSTALLED	5,619	0.79	0.44	3,470	0.35	0.28	34,549	0.74	0.63
CONTINGENCY, 25%	1,405	0.79	0.44	867	0.35	0.28	8,637	0.74	0.63
BATTERY LIMITS INVESTMENT	7,024	0.79	0.44	4,337	0.35	0.28	43,186	0.74	0.63
OFFSITES, INSTALLED									
CLARIFIED WATER	100	0.74	0.74	5	0.74	0.74	449	0.74	0.74
COOLING WATER	443	0.92	0.92	24	0.92	0.92	2,075	0.92	0.92
PROCESS WATER	63	0.62	0.62	3	0.62	0.62	293	0.62	0.62
BOILER FEED WATER	260	0.57	0.51	3	0.24	0.00	890	0.55	0.47
STEAM	1,842	0.95	0.80	8	0.74	0.31	6,030	0.94	0.78
REFRIGERATION	--	--	--	48	0.95	0.71	--	--	--
INERT GAS	22	0.52	0.52	--	--	--	34	0.52	0.52
TANKAGE	--	--	--	--	--	--	457	0.65	0.65
UTILITIES & STORAGE	2,730	0.89	0.78	90	0.89	0.69	10,228	0.88	0.76

Table 6.23
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

PRODUCTION COSTS

PEP COST INDEX: 624

VARIABLE COSTS

	UNIT COST	CONSUMPTION PER LB	\$/LB
<hr/>			
RAW MATERIALS			
HYDROGEN	0.388 ¢/FT^3	12.567 FT^3	4.88
BUTADIENE	13 ¢/LB	0.54476 LB	7.08
HYDROGEN CYANIDE	46.18 ¢/LB	0.54255 LB	25.05
AMMONIA	8.75 ¢/LB	0.00166 LB	0.01
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.00343 LB	0.96
SOIDUM BISULFITE	19.25 ¢/LB	0.10992 LB	2.12
SOIDUM SULFITE	30.5 ¢/LB	0.06672 LB	2.03
TRIPHYPHENYLBORANE	10.26 \$/LB	0.00012 LB	0.12
PHOSPHOROUS TRICHLORIDE	49 ¢/LB	0.0002 LB	0.01
CARBON DIOXIDE	3.24 ¢/LB	0.00166 LB	0.01
IRON CATALYST	110 ¢/LB	0.006 LB	0.66
CYCLOHEXANE	15.3 ¢/LB	0.00059 LB	0.01
NICKEL POWDER	8.5 \$/LB	0.00039 LB	0.33
<hr/>			
GROSS RAW MATERIALS			43.27
<hr/>			
BY-PRODUCTS			
HEXAMETHYLENEIMINE	2.21 \$/LB	-0.004 LB	-0.88
HEAVY AMINE	35 ¢/LB	-0.013 LB	-0.46
<hr/>			
TOTAL BY-PRODUCTS			-1.34
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	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG	
<hr/>				
UTILITIES				
COOLING WATER	7.45 ¢/MGAL	46.4 GAL	387 LITERS	0.35
PROCESS WATER	1.101 \$/MGAL	0.147 GAL	1.22 LITERS	0.02
STEAM, 150 PSIG	4.51 \$/MLB	2.2 LB	2.2 KG	0.99
STEAM, 600 PSIG	5.72 \$/MLB	6.26 LB	6.26 KG	3.58
ELECTRICITY	4 ¢/KWH	0.151 KWH	0.332 KWH	0.60
NATURAL GAS	3.24 \$/MMBTU	78.8 BTU	43.8 KCAL	0.03
INERT GAS, LOW P	0.51 \$/MSCF	0.197 SCF	12.3 LITERS	0.01
REFRIGERATION, 40°F	5.02 ¢/TON-HR	0.0211 TON-HR	0.164 KWH	0.11
<hr/>				
TOTAL UTILITIES				5.69

Table 6.23 (Concluded)
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

PRODUCTION COSTS

PEP COST INDEX: 624

CAPACITY (MILLION LB/YR)*	100	200#	400
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	68.0	95.0	144.8
OFFSITES	40.6	61.2	102.4
TOTAL FIXED CAPITAL (TFC)	108.6	156.3	247.2
SCALING EXPONENTS	0.53	0.66	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	43.27	43.27	43.27
BY-PRODUCTS	-1.34	-1.34	-1.34
UTILITIES	5.69	5.69	5.69
VARIABLE COSTS	47.62	47.62	47.62
OPERATING LABOR, 12/SHIFT, \$33.58/HR	3.53	1.76	0.88
MAINTENANCE LABOR, 3%/YR OF BLI	2.04	1.43	1.09
CONTROL LAB LABOR, 20% OF OPER LABOR	0.71	0.35	0.18
LABOR COSTS	6.28	3.54	2.15
MAINTENANCE MATERIALS, 3%/YR OF BLI	2.04	1.43	1.09
OPERATING SUPPLIES, 10% OF OPER LABOR	0.35	0.18	0.09
TOTAL DIRECT COSTS	56.29	52.77	50.95
PLANT OVERHEAD, 80% OF LABOR COSTS	5.02	2.83	1.72
TAXES AND INSURANCE, 2%/YR OF TFC	2.17	1.56	1.24
PLANT CASH COSTS	63.48	57.16	53.91
DEPRECIATION, 10%/YR OF TFC	10.86	7.81	6.18
PLANT GATE COSTS	74.34	64.97	60.09
G&A, SALES, RESEARCH	9.00	9.00	9.00
NET PRODUCTION COST	83.34	73.97	69.09
ROI BEFORE TAXES, 25%/YR OF TFC	27.15	19.53	15.45
PRODUCT VALUE	110.49	93.50	84.54

* OF HMDA

BASE CASE

HMDA AND CAPM FROM BUTADIENE VIA ADIPONITRILE

This process is same as the process described in Section 5 of this report, which produces both HMDA and CAPM on an equal amount basis.

Cost Estimates

The economics for this process is same as those given in Tables 5.26 and 5.27 except that CAPM is credited as a by-product in this integrated process. At a capacity of 330 million lb/yr (150,000 t/yr), the production costs are summarized in Table 6.24.

With a unit price of butadiene at 13 ¢/lb, and CAPM is credited at 84 ¢/lb, the cash cost and the plant gate cost for HMDA are estimated at 33.5 ¢/lb and 47.9 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for HMDA is estimated at 93 ¢/lb.

Table 6.24
HMDA AND CAPROLACTAM FROM BUTADIENE VIA ADN
BY HYDROCYANATION, HYDROGENATION AND CYCLIZATION

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
BUTADIENE	13 ¢/LB	1.13112 LB	14.70
AMMONIA	8.75 ¢/LB	0.00364 LB	0.03
HYDROGEN (97%)	0.388 ¢/FT^3	20.0358 FT^3	7.77
ETHANOL	155 ¢/GALLON	0.00252 GALLON	0.39
HYDROGEN CYANIDE	46.18 ¢/LB	1.12652 LB	52.02
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.00712 LB	1.99
SODIUM BISULFITE	19.25 ¢/LB	0.22824 LB	4.39
SODIUM SULFITE	30.5 ¢/LB	0.13854 LB	4.23
TRIPHENYLBORANE	10.26 \$/LB	0.00026 LB	0.27
PHOSPHORUS TRICHLORIDE	49 ¢/LB	0.0004 LB	0.02
CYCLOHEXANE	15.62 ¢/LB	0.00122 LB	0.02
NICKEL POWDER	8.79 \$/LB	0.00082 LB	0.72
GROSS RAW MATERIALS			86.55
BY-PRODUCTS			
LIGHT ENDS AS FUEL	2.21 \$/MMBTU	-0.00132 MMBTU	-0.29
CAPM	84.03 ¢/LB	-1 LB	-84.03
TOTAL BY-PRODUCTS			-84.32
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	95.2 GAL	794 LITERS
PROCESS WATER	1.101 \$/MGAL	0.387 GAL	3.23 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	4.78 LB	4.78 KG
STEAM, 600 PSIG	5.72 \$/MLB	15 LB	15 KG
STEAM, 1500 PSIG	6.16 \$/MLB	9.53 LB	9.53 KG
ELECTRICITY	4 ¢/KWH	0.102 KWH	0.225 KWH
NATURAL GAS	3.24 \$/MMBTU	167 BTU	92.9 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.263 SCF	16.4 LITERS
REFRIGERATION, 20°F	5.08 ¢/TON-HR	0.571 TON-HR	4.43 KWH
REFRIGERATION, 40°F	5 ¢/TON-HR	0.044 TON-HR	0.341 KWH
TOTAL UTILITIES			20.94

Table 6.24 (Concluded)
HMDA AND CAPROLACTAM FROM BUTADIENE VIA ADN
BY HYDROCYANATION, HYDROGENATION AND CYCLIZATION

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	165	330#	660
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	139.1	195.7	294.4
OFFSITES	160.9	280.9	505.4
-----	-----	-----	-----
TOTAL FIXED CAPITAL (TFC)	299.9	476.6	799.8
SCALING EXPONENTS		0.67	0.75
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	86.55	86.55	86.55
BY-PRODUCTS	-84.32	-84.32	-84.32
UTILITIES	20.94	20.94	20.94
-----	-----	-----	-----
VARIABLE COSTS	23.17	23.17	23.17
OPERATING LABOR, 12/SHIFT, \$33.58/HR	2.14	1.07	0.53
MAINTENANCE LABOR, 3%/YR OF BLI	2.53	1.78	1.34
CONTROL LAB LABOR, 20% OF OPER LABOR	0.43	0.21	0.11
-----	-----	-----	-----
LABOR COSTS	5.10	3.06	1.98
MAINTENANCE MATERIALS, 3%/YR OF BLI	2.53	1.78	1.34
OPERATING SUPPLIES, 10% OF OPER LABOR	0.21	0.11	0.05
-----	-----	-----	-----
TOTAL DIRECT COSTS	31.01	28.12	26.54
PLANT OVERHEAD, 80% OF LABOR COSTS	4.08	2.45	1.58
TAXES AND INSURANCE, 2%/YR OF TFC	3.64	2.89	2.42
-----	-----	-----	-----
PLANT CASH COSTS	38.73	33.46	30.54
DEPRECIATION, 10%/YR OF TFC	18.18	14.44	12.12
-----	-----	-----	-----
PLANT GATE COSTS	56.91	47.90	42.66
G&A, SALES, RESEARCH	9.00	9.00	9.00
-----	-----	-----	-----
NET PRODUCTION COST	65.91	56.90	51.66
ROI BEFORE TAXES, 25%/YR OF TFC	45.45	36.10	30.29
-----	-----	-----	-----
PRODUCT VALUE	111.36	93.00	81.95

* OF HMDA

BASE CASE

NYLON 66 RESINS BY THE CONTINUOUS PROCESS

Process Description

Figure 6.5 (foldout at end of report) presents the flow diagram for this process, and the utilities summary and major equipment list are given in Table 6.25 and 6.26, respectively. A brief description of the process is given below.

The process shown below is based on a patent assigned to BASF. Adipic acid is dissolved in deionized water at 95°C to form a 52% solution. This is mixed with a recycled stream of nylon salt (hexamethylene diammonium adipate) solution, which has been previously mixed with molten hexamethylenediamine (HMDA), slightly below the stoichiometric requirement. Then, a solution of HMDA in water, in an amount controlled by the pH of the mixed stream, is added to exact stoichiometry. The mixed stream is cooled to remove the heat of neutralization. Most of it is recycled, and a small part is withdrawn as product, 63% nylon salt solution in water.

The nylon salt solution is heated at 232°C and 18.0 atm to evaporate most of the water and partially polycondense the nylon salt to a low molecular weight polymer. The polycondensation continues in tubular reactors at 232-285°C and 18.0 atm inlet/4.4 atm outlet. Water vapor is released in a subsequent separation. Finally, the molten mass is heated in a finishing reactor at 271°C under vacuum to attain the desired degree of polymerization. The melt is extruded into strands, which are pelletized, dried, and packed in to 55 lb bags. Overall loss is 0.5%. The above process is for manufacturing natural color unmodified resin for injection molding. At present, all major nylon 66 producers use a continuous process.

Economics

Capital investment summary for this process is given in Table 6.27, and those for operation sections are listed in Table 6.28. At a capacity of 135 million lb/yr (61,200 t/yr), the process requires \$48.2 million for the battery limits and \$72.7 million for total fixed capital.

The production costs are summarized in Table 6.29. With a unit price of ADA at 62.5 ¢/lb and that of HMDA at 90 ¢/lb, the cash cost and the plant gate cost for nylon 66 resin are estimated at 95.4 ¢/lb and 100.8 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for nylon 66 resin is estimated at 129.3 ¢/lb.

Table 6.25
NYLON 66 RESIN BY CONTINUOUS PROCESS

UTILITIES SUMMARY					
		BATTERY LIMITS	SECTION	SECTION	SECTION
	UNITS	TOTAL	100	200	300
AVERAGE CONSUMPTIONS					
COOLING WATER	GPM	2,403	351	1,796	256
PROCESS WATER	GPM	27	27	--	--
ELECTRICITY	KW	2,332	370	351	1,612
INERT GAS, LOW P	M SCF/HR	19	7	12	--
STEAM, 150 PSIG	M LB/HR	46	27	19	--

Table 6.26
NYLON 66 RESIN BY CONTINUOUS PROCESS

MAJOR EQUIPMENT				
CAPACITY: 135 MILLION LB/YR (61,200 T/YR) NYLON 66 RESIN AT 0.90 STREAM FACTOR				
EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
REACTORS				
R-101	REACTOR	3000 GAL	CLADDING: 304 SS AGITATOR: 304 SS	WITH 15 HP TURBINE AGITATOR
R-201 R-202A,B	EVAPORATIVE REACTOR TUBULAR REACTORS	10,800 GAL 3,200 SQ FT EA 27 MMBTU/HR	CLADDING: 304 SS SHELL: C.S. TUBES: 304 SS	JACKETED AND INNER PARTITION
R-203	FINISHING REACTOR	9,200 GAL	CLADDING: 304 SS	
COLUMNS				
C-201A,B	ADSORBERS	3.5 FT DIA EA 15 FT	CLADDING: 304 SS PACKING: SILICA GEL	10 FT OF PACKING
HEAT EXCHANGERS				
E-101	COOLER	700 SQ FT 3.5 MMBTU/HR	SHELL: C.S. TUBES: 304 SS	
E-201	CONDENSER	680 SQ FT 9.2 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
E-202	CONDENSER	220 SQ FT 3.9 MMBTU/HR	SHELL: C.S. TUBES: C.S.	
TANKS				
T-101	HMDA TANK	30,000 GAL	304 SS	WITH HEATING COILS
T-102	ADIPIC ACID BIN	189,000 GAL	304 SS	
T-103	DEIONIZED WATER TANK	35,000 GAL	C.S.	
T-104A,B	NYLON SALT SOLUTION TANKS	41,000 GAL EA	304 SS	WITH HEATING COILS
T-151A-C	HMDA STORAGE	56,000 GAL EA	304 SS	WITH HEATING COILS, NOT SHOWN IN FLOW DIAGRAM
T-201	ACETIC ACID TANK	5,400 GAL	316 SS	
T-202	ADDITIVE TANK	5,400 GAL	304 SS	
T-203	ADDITIVE TANK	5,400 GAL	304 SS	
T-204	ADDITIVE TANK	5,400 GAL	304 SS	
T-205	WASTE WATER TANK	27,000 GAL	C.S.	
PRESSURE VESSELS				
V-101A,B	ADIPIC ACID DISSOLVERS	13,500 GAL EA	304 SS CLAD	EACH EQUIPPED WITH 50 HP TURBINE AGITATOR
V-102A,B	HMDA DISSOLVERS	2,700 GAL EA	304 SS CLAD	EACH EQUIPPED WITH 10 HP TURBINE AGITATOR
V-201	ACETIC ACID VESSEL	110 GAL	304 SS	WITH 1 HP TURBINE AGITATOR
V-202	CONDENSATE RECIEVER	270 GAL	304 SS	
V-203	CONDENSATE RECIEVER	190 GAL	304 SS	
MISCELLANEOUS EQUIPMENT				
M-101A-C	SCREW CONVEYOR	8200 LB/HR EA	304 SS	
M-102A-C	STATIC MIXER	410000 LB/HR EA	304 SS	
M-103A-C	STATIC MIXER	418000 LB/HR EA	304 SS	
M-104A-C	STATIC MIXER	180 LB/HR EA	304 SS	
M-201A-C	FILTER	3860 LB/HR EA	316 SS	CARTRIDGE FILTER
M-202A-C	STATIC MIXER	3855 LB/HR EA	304 SS	
M-203	VACUUM SYSTEM [*]	300 mmHG	CARBON STEEL	NOT SHOWN IN FLOW DIAGRAM

Table 6.26 (Concluded)
NYLON 66 RESIN BY CONTINUOUS PROCESS

MAJOR EQUIPMENT

CAPACITY: 135 MILLION LB/YR (61,200 T/YR)
 NYLON 66 RESIN
 AT 0.90 STREAM FACTOR

EQUIPMENT NUMBER	NAME	SIZE	MATERIAL OF CONSTRUCTION	REMARKS
SPECIAL EQUIPMENT				
S-201A-C	PELLETIZER AND ASSOC.	7750 LB/HR EA	304 SS	
PACKAGE UNITS				
G-101	DEIONIZED WATER SYSTEM	300000 LB/DAY	CARBON STEEL	
G-301A-C	RESIN SURGE HOPPERS	24 CUFT EA	ALUMINUM	
G-302A-C	PRODUCT SCREENS	5-10 MESH	CARBON STEEL	
G-303A-C	SURGE BINS	1540 CUFT EA	EPOXY LINED	
G-304A-C	RESIN FEED HOPPERS	78 CUFT EA	ALUMINUM	
G-305A-C	WEIGH BELT FEEDERS	5740 LB/HR EA	304 SS	
G-306A-C	SCALE HOPPERS	300 DIAL EA	ALUMINUM	
G-307A-C	SCALE HOPPERS	300 DIAL EA	ALUMINUM	
G-308A-C	RIBBON BLENDERS	60 CUFT EA	304 SS	
G-309A-C	ADDITIONAL FEED BINS	190 CUFT EA	EPOXY LINED	
G-310A-C	WEIGH BELT FEEDERS	570 LB/HR EA	304 SS	
G-311A-C	EXTRUDER-PELLETIZERS	2540 LB/HR EA	304 SS	
G-312A-F	RUN BINS	170 CUFT EA	EPOXY LINED	
G-313A-C	BLENDING BINS	1530 LB/HR EA	EPOXY LINED	
G-314A-J	STORAGE BINS	6000 CUFT EA	EPOXY LINED	
G-315A-E	LOADING AND PACKAGING	15 BAGS/MIN EA	304 SS	
G-316	PNEUMATIC CONVEYOR SYSTEM		ALUMINUM	
PUMPS				
SECTION	OPERATING	SPARES	OPERATING BHP	
100	13	10	22	
200	8	8	13	

Table 6.27
NYLON 66 RESIN BY CONTINUOUS PROCESS

TOTAL CAPITAL INVESTMENT			
CAPACITY: 135 MILLION LB/YR (61,200 T/YR)			
NYLON 66 RESIN			
AT 0.90 STREAM FACTOR			
PEP COST INDEX: 624			
	COST (\$1,000)	CAPACITY EXPONENT	
		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.			
REACTORS	1,121	0.69	0.66
COLUMNS	79	0.63	0.50
VESSELS & TANKS	2,385	0.69	0.58
HEAT EXCHANGERS	93	0.70	0.70
SPECIAL EQUIPMENT	657	0.54	0.51
MISCELLANEOUS EQUIPMENT	182	0.59	0.56
PUMPS	571	0.35	0.25

TOTAL	5,088	0.63	0.55
DIRECT INSTALLATION COSTS	8,519	0.35	0.32
COMPOUNDING UNITS	7,893	0.72	0.72
BULK HANDLING UNITS	2,480	0.69	0.69
DEIONIZED WATER SYSTEM	1,710	0.39	0.31
INDIRECT COSTS	9,393	0.51	0.46
UNSCHEDULED EQUIPMENT, 10%	3,508	0.55	0.50

BATTERY LIMITS, INSTALLED	38,591	0.55	0.50
CONTINGENCY, 25%	9,648	0.55	0.50

BATTERY LIMITS INVESTMENT	48,239	0.55	0.50
OFF-SITES, INSTALLED			
CLARIFIED WATER	262	0.40	0.40
COOLING WATER	500	0.92	0.92
PROCESS WATER	162	0.40	0.40
BOILER FEED WATER	512	0.40	0.40
STEAM	1,563	0.60	0.60
INERT GAS	224	0.52	0.52
TANKAGE	884	0.79	0.70
WAREHOUSE FACILITIES	2,149	0.65	0.65

UTILITIES & STORAGE	6,255	0.64	0.62
GENERAL SERVICE FACILITIES	10,899	0.56	0.51
WASTE TREATMENT	2,412	0.55	0.50

TOTAL	19,566	0.59	0.54
CONTINGENCY, 25%	4,892	0.59	0.54

OFF-SITES INVESTMENT	24,458	0.59	0.54
TOTAL FIXED CAPITAL	72,697	0.56	0.51

Table 6.28
NYLON 66 RESIN BY CONTINUOUS PROCESS

CAPITAL INVESTMENT BY SECTION

CAPACITY: 135 MILLION LB/YR (61,200 T/YR)
 NYLON 66 RESIN
 AT 0.90 STREAM FACTOR

PEP COST INDEX: 624

NYLON SALT AQUEOUS SOLUTION PREPARATIONPOLYCONDENSATION AND RESIN FORMATIONRESIN COMPOUNDING AND FINISHING

	CAPACITY EXPONENT			CAPACITY EXPONENT			CAPACITY EXPONENT		
	COST (\$1,000)			COST (\$1,000)			COST (\$1,000)		
		UP	DOWN		UP	DOWN		UP	DOWN
BATTERY LIMITS EQUIPMENT, F.O.B.									
REACTORS	140	0.50	0.48	981	0.71	0.69	--	--	--
COLUMNS	--	--	--	79	0.63	0.50	--	--	--
VESSELS & TANKS	1,778	0.62	0.57	607	0.87	0.62	--	--	--
HEAT EXCHANGERS	47	0.78	0.79	46	0.61	0.61	--	--	--
SPECIAL EQUIPMENT	--	--	--	657	0.54	0.51	--	--	--
MISCELLANEOUS EQUIPMENT	53	0.58	0.50	129	0.59	0.58	--	--	--
PUMPS	436	0.35	0.24	136	0.36	0.29	--	--	--
TOTAL	2,453	0.57	0.50	2,635	0.68	0.59	--	--	--
DIRECT INSTALLATION COSTS	5,122	0.36	0.33	3,397	0.33	0.31	--	--	--
COMPOUNDING UNITS	--	--	--	--	--	--	7,893	0.72	0.72
BULK HANDLING UNITS	--	--	--	--	--	--	2,480	0.69	0.69
DEIONIZED WATER SYSTEM	1,710	0.39	0.31	--	--	--	--	--	--
INDIRECT COSTS	3,395	0.37	0.32	2,205	0.44	0.37	3,792	0.66	0.66
UNSCHEDULED EQUIPMENT, 10%	1,268	0.41	0.36	824	0.48	0.41	1,417	0.70	0.70
BATTERY LIMITS INSTALLED	13,948	0.41	0.36	9,062	0.48	0.41	15,582	0.70	0.70
CONTINGENCY, 25%	3,487	0.41	0.36	2,265	0.48	0.41	3,896	0.70	0.70
BATTERY LIMITS INVESTMENT	17,434	0.41	0.36	11,327	0.48	0.41	19,478	0.70	0.70
OFFSITES, INSTALLED									
CLARIFIED WATER	96	0.40	0.40	147	0.40	0.40	19	0.40	0.40
COOLING WATER	73	0.92	0.92	374	0.92	0.92	53	0.92	0.92
PROCESS WATER	18	0.40	0.40	94	0.40	0.40	13	0.40	0.40
BOILER FEED WATER	301	0.40	0.40	211	0.40	0.40	--	--	--
STEAM	919	0.60	0.60	643	0.60	0.60	--	--	--
INERT GAS	80	0.52	0.52	144	0.52	0.52	--	--	--
TANKAGE	884	0.79	0.70	--	--	--	--	--	--
WAREHOUSE FACILITIES	2,149	0.65	0.65	--	--	--	--	--	--
UTILITIES & STORAGE	4,521	0.65	0.63	1,613	0.62	0.60	86	0.75	0.70

Table 6.29
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
ADIPIC ACID	62.5 ¢/LB	0.646538 LB	40.41
HEXAMETHYLENE DIAMINE	90 ¢/LB	0.517043 LB	46.53
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05

GROSS RAW MATERIALS			86.99
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	8.42 GAL	70.3 LITERS
PROCESS WATER	1.101 \$/MGAL	0.0946 GAL	0.79 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	2.68 LB	2.68 KG
ELECTRICITY	4 ¢/KWH	0.136 KWH	0.3 KWH
INERT GAS, LOW P	0.51 \$/MSCF	1.1 SCF	68.9 LITERS

TOTAL UTILITIES			1.88

Table 6.29 (Concluded)
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	68	135#	270
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	34.1	48.2	70.7
OFFSITES	16.8	24.5	36.8
-----	-----	-----	-----
TOTAL FIXED CAPITAL (TFC)	50.9	72.7	107.5
SCALING EXPONENTS	0.51	0.56	
PRODUCTION COSTS (¢/LB)			
RAW MATERIALS	86.99	86.99	86.99
UTILITIES	1.88	1.88	1.88
-----	-----	-----	-----
VARIABLE COSTS	88.87	88.87	88.87
OPERATING LABOR, 5/SHIFT, \$33.58/HOUR	2.18	1.09	0.54
MAINTENANCE LABOR, 3%/YR OF BLI	1.52	1.07	0.79
CONTROL LAB LABOR, 20% OF OPER LABOR	0.44	0.22	0.11
-----	-----	-----	-----
LABOR COSTS	4.14	2.38	1.44
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.52	1.07	0.79
OPERATING SUPPLIES, 10% OF OPER LABOR	0.22	0.11	0.05
-----	-----	-----	-----
TOTAL DIRECT COSTS	94.75	92.43	91.15
PLANT OVERHEAD, 80% OF LABOR COSTS	3.31	1.90	1.15
TAXES AND INSURANCE, 2%/YR OF TFC	1.51	1.08	0.80
-----	-----	-----	-----
PLANT CASH COSTS	99.57	95.41	93.10
DEPRECIATION, 10%/YR OF TFC	7.54	5.38	3.98
-----	-----	-----	-----
PLANT GATE COSTS	107.11	100.79	97.08
G&A, SALES, RESEARCH	15.00	15.00	15.00
-----	-----	-----	-----
NET PRODUCTION COST	122.11	115.79	112.08
ROI BEFORE TAXES, 25%/YR OF TFC	18.85	13.46	9.95
-----	-----	-----	-----
PRODUCT VALUE	140.96	129.25	122.03

* OF NYLON 66 RESIN

BASE CASE

7 ECONOMICS FOR STRATEGIC BUSINESS UNITS FOR NYLON 6 AND NYLON 66

INTRODUCTION

In this section, we present economics of strategic units (SBUs) for the production of nylon 6 and nylon 66 resins. There are four configurations of SBUs considered in this section for nylon 6 chips production as summarized below:

- N6-SBU1—Integration of cyclohexane-based NOx process with continuous process for nylon 6 chips
- N6-SBU2—Integration of cyclohexane-based HPO process with continuous process for nylon 6 chips
- N6-SBU3—Integration of phenol-based HPO process with continuous process for nylon 6 chips
- N6-SBU4—Integration of butadiene-based CAPM process via amino-caproate with continuous process for nylon 6 chips
- N6-SBU5—Integration of butadiene-based CAPM/HMDA process via adiponitrile with continuous process for nylon 6 chips

For the production of nylon 66 resins, also five configurations of SBUs are considered in this section; they are:

- N66-SBU1—Integration of cyclohexane-based ADA oxidation process and butadiene-based HMDA hydrocyanation process with continuous process for nylon 66 resins
- N66-SBU2—Integration of Butadiene-based ADA carbalkoxylation process and butadiene-based HMDA hydrocyanation process with continuous process for nylon 66 resins
- N66-SBU3—Integration of benzene-based ADA process and butadiene-based HMDA hydrocyanation process with continuous process for nylon 66 resins
- N66-SBU4—Integration of cyclohexane-based ADA oxidation process and adiponitrile-based HMDA process with continuous process for nylon 66 resins
- N66-SBU5—Integration of butadiene-based CAPM/HMDA process via adiponitrile with continuous process for nylon 66 resins

In each of aforementioned SBUs, the determination of configuration and production capacity is based on the information presented in Section 3 of this report. In industry practice, the production capacities for nylon precursors are, in most cases, planned to accommodate the demands for downstream production of both nylon resins and nylon fibers. We will discuss and compare the economics of SBUs with the economics of a stand-alone nylon production with captive precursor(s). In actual practice, the precursors, if not integrated produced, can be obtained either captively or from an allied company.

STRATEGIC UNITS FOR THE PRODUCTION OF NYLON 6 CHIPS

N6-SBU1 Description

The configuration of this SBU is determined with the status of BASF's CAPM and nylon 6 chips production in Western Europe in mind. BASF has both CAPM and nylon 6 production at Ludwigshafen, Germany with production capacities of 331 million lb/yr (150,000 t/yr) and 154 million lb/yr (70,000 t/yr), respectively. The company also has production of CAPM and nylon 6 resin at Antwerpen, Belgian with production capacities of 595 million lb/yr (270,000 t/yr) and 132 million lb/yr (60,000 t/yr), respectively. The nylon 6 production in this case is 154 million lb/yr (70,000 t/yr) and the CAPM production capacity is scaled down from 331 million lb/yr (150,000 t/yr) to matched the nylon production. The price of captive CAPM used in a stand-alone nylon 6 plant is derived from the 331 million lb/yr (150,000 t/yr) plant, which employs a cyclohexane-based CAPM NOx process.

N6-SBU1 Cost Estimates

Table 7.1 presents the economics of N6-SBU1. The battery limits for the integrated unit is estimated at \$200.2 million and total fixed capital is \$331.9 million. With a unit price of cyclohexane at 15.62 ¢/lb, the cash cost and the plant gate cost for nylon 6 are estimated at 67.4 ¢/lb and 88.9 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 154.6 ¢/lb.

As mentioned earlier, the production capacity for CAPM is greater than that of nylon 6. In the present case, the CAPM production capacity is 331 million lb/yr (150,000 t/yr). There are various ways to determine the price of captive CAPM used for a stand-alone nylon 6 plant of 154 million lb/yr (70,000 t/yr). It can be either the cash cost or plant gate cost plus transportation cost, if there is any. For simplicity, we select the production cost of 71.5 ¢/lb for the captive CAPM for the stand-alone nylon 6 plant. The resulting economics is given in Table 7.2.

Table 7.2 indicates that the product value for nylon 6 is reduced by about 24% to 116.8 ¢/lb when CAPM is captively derived from a large precursor plant.

N6-SBU2 Description

The configuration of this SBU is determined with the status of DSM's CAPM and nylon 6 resin production in the United States in mind. The CAPM plant at Augusta, GA has a capacity of 430 million lb/yr (195,000 t/yr), while the nylon 6 plant at that location is small at 33 million lb/yr (15,000 t/yr). The nylon 6 production in the present configuration is hypothetically assumed at 154 million lb/yr (70,000 t/yr) and the CAPM production capacity is scaled down from 430 million lb/yr (195,000 t/yr) to matched the nylon production. In the case of a stand-alone nylon 6 resin plant, the unit price of captive CAPM is derived from the 430 million lb/yr (195,000 t/yr) plant, which uses a cyclohexane-based CAPM HPO process.

N6-SBU2 Cost Estimates

Table 7.3 presents the economics of N6-SBU2. The battery limits for the integrated unit is estimated at \$244.4 million and total fixed capital is \$395.8 million. With a unit price of cyclohexane at 15.62 ¢/lb, the cash cost and the plant gate cost for nylon 6 are estimated at 75 ¢/lb and 100.6 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 176.7 ¢/lb.

In the present case, the price of captive CAPM produced by the 331 million lb/yr (150,000 t/yr) plant is estimated at 79.3 ¢/lb. The economics of a stand-alone nylon 6 plant of 154 million lb/yr (70,000 t/yr) with this CAPM price are then generated and given in Table 7.4. It appears that the product value for nylon 6 is reduced by about 30% to 124.2 ¢/lb when CAPM is captively derived from a large precursor plant.

Table 7.1
ECONOMICS OF N6-SBU1

PRODUCTION COSTS

PEP COST INDEX: 624

VARIABLE COSTS

	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
ACETIC ACID	31 ¢/LB	0.001156 LB	0.04
AMMONIA	8.75 ¢/LB	0.57194 LB	5.00
BENZENE	9.5 ¢/LB	0.007778 LB	0.07
CAUSTIC SODA	11 ¢/LB	0.122684 LB	1.35
COBALT NAPHTHENATE	3.71 \$/LB	0.000076 LB	0.03
COBALTOUS SULFATE	2.81 \$/LB	0.000095 LB	0.03
CYCLOHEXANE	15.62 ¢/LB	0.972984 LB	15.20
HYDROGEN	0.388 ¢/FT^3	0.006549 FT^3	NEGL
NYLON 6 SCARP	64.5 ¢/LB	0.06493 LB	4.19
OLEUM (32%)	4.01 ¢/LB	1.11586 LB	4.47
OXYGEN	2.017 ¢/LB	0.347006 LB	0.70
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
OTHER CHEMICALS	1 ¢/LB	0.02 LB	0.02
GROSS RAW MATERIALS			31.31
BY-PRODUCTS			
AMMONIUM SULFATE	1.9 ¢/LB	-1.60539 LB	-3.05
FUEL	2.21 \$/MMBTU	-0.00095 MMBTU	-0.21
NITRIC ACID (DILUTE)	4.9 ¢/LB	-0.041348 LB	-0.20
TOTAL BY-PRODUCTS			-3.46
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	146 GAL	1,220 LITERS
PROCESS WATER	1.101 \$/MGAL	0.598 GAL	4.99 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	9.55 LB	9.55 KG
STEAM, 600 PSIG	5.72 \$/MLB	12.6 LB	12.6 KG
STEAM, 1500 PSIG	6.16 \$/MLB	3.88 LB	3.88 KG
ELECTRICITY	4 ¢/KWH	0.334 KWH	0.736 KWH
NATURAL GAS	3.24 \$/MMBTU	613 BTU	341 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	1.28 SCF	79.7 LITERS
REFRIGERATION, 40°F	4.99 ¢/TON-HR	0.145 TON-HR	1.13 KWH
TOTAL UTILITIES			17.42

Table 7.1 (Concluded)
ECONOMICS OF N6-SBU1

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	77	154#	309
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	148.6	200.2	296.4
OFFSITES	86.4	131.7	217.6
-----	-----	-----	-----
TOTAL FIXED CAPITAL (TFC)	235.0	331.9	514.0
SCALING EXPONENTS	0.50	0.63	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	31.31	31.31	31.31
BY-PRODUCTS	-3.46	-3.46	-3.46
UTILITIES	17.42	17.42	17.42
-----	-----	-----	-----
VARIABLE COSTS	45.27	45.27	45.27
OPERATING LABOR, 16/SHIFT, \$33.58/HR	6.10	3.05	1.52
MAINTENANCE LABOR, 3%/YR OF BLI	5.78	3.89	2.88
CONTROL LAB LABOR, 20% OF OPER LABOR	1.22	0.61	0.30
-----	-----	-----	-----
LABOR COSTS	13.10	7.55	4.70
MAINTENANCE MATERIALS, 3%/YR OF BLI	5.78	3.89	2.88
OPERATING SUPPLIES, 10% OF OPER LABOR	0.61	0.30	0.15
-----	-----	-----	-----
TOTAL DIRECT COSTS	64.76	57.01	53.00
PLANT OVERHEAD, 80% OF LABOR COSTS	10.48	6.04	3.76
TAXES AND INSURANCE, 2%/YR OF TFC	6.09	4.30	3.33
-----	-----	-----	-----
PLANT CASH COSTS	81.33	67.35	60.09
DEPRECIATION, 10%/YR OF TFC	30.45	21.51	16.66
-----	-----	-----	-----
PLANT GATE COSTS	111.78	88.86	76.75
G&A, SALES, RESEARCH	12.00	12.00	12.00
-----	-----	-----	-----
NET PRODUCTION COST	123.78	100.86	88.75
ROI BEFORE TAXES, 25%/YR OF TFC	76.13	53.77	41.64
-----	-----	-----	-----
PRODUCT VALUE	199.91	154.63	130.39

* OF NYLON 6 CHIPS

BASE CASE

Table 7.2
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	\$/LB
RAW MATERIALS			
CAPROLACTAM	71.5 ¢/LB	0.94769 LB	67.76
NYLON 6 SCRAP	64.5 ¢/LB	0.06493 LB	4.19
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
CAUSTIC SODA	11 ¢/LB	0.00373 LB	0.04
OTHER CHEMICALS	-- ¢/LB	-- LB	0.02
GROSS RAW MATERIALS			72.22
UTILITIES			
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
COOLING WATER	7.45 ¢/MGAL	25.5 GAL	213 LITERS
PROCESS WATER	1.101 \$/MGAL	0.0343 GAL	0.287 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	1.07 LB	1.07 KG
STEAM, 600 PSIG	5.72 \$/MLB	1.17 LB	1.17 KG
STEAM, 1500 PSIG	6.16 \$/MLB	3.86 LB	3.86 KG
ELECTRICITY	4 ¢/KWH	0.145 KWH	0.321 KWH
NATURAL GAS	3.24 \$/MMBTU	250 BTU	139 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.143 SCF	8.93 LITERS
TOTAL UTILITIES			4.39

Table 7.2 (Concluded)
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	77	154#	309
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	40.1	56.2	83.1
OFFSITES	27.7	41.5	64.4
TOTAL FIXED CAPITAL (TFC)	67.8	97.7	147.5
SCALING EXPONENTS	0.53	0.59	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	72.22	72.22	72.22
UTILITIES	4.39	4.39	4.39
VARIABLE COSTS	76.61	76.61	76.61
OPERATING LABOR, 4/SHIFT, \$33.58/HR	1.52	0.76	0.38
MAINTENANCE LABOR, 3%/YR OF BLI	1.56	1.09	0.81
CONTROL LAB LABOR, 20% OF OPER LABOR	0.30	0.15	0.08
LABOR COSTS	3.38	2.00	1.27
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.56	1.09	0.81
OPERATING SUPPLIES, 10% OF OPER LABOR	0.15	0.08	0.04
TOTAL DIRECT COSTS	81.70	79.78	78.73
PLANT OVERHEAD, 80% OF LABOR COSTS	2.70	1.60	1.02
TAXES AND INSURANCE, 2%/YR OF TFC	1.76	1.27	0.96
PLANT CASH COSTS	86.16	82.65	80.71
DEPRECIATION, 10%/YR OF TFC	8.78	6.33	4.78
PLANT GATE COSTS	94.94	88.98	85.49
G&A, SALES, RESEARCH	12.00	12.00	12.00
NET PRODUCTION COST	106.94	100.98	97.49
ROI BEFORE TAXES, 25%/YR OF TFC	21.96	15.83	11.95
PRODUCT VALUE	128.90	116.81	109.44

* OF NYLON 6 CHIPS

BASE CASE

Table 7.3
ECONOMICS OF N6-SBU2

PRODUCTION COSTS

PEP COST INDEX: 624

VARIABLE COSTS

	UNIT COST	CONSUMPTION PER LB	\$/LB
<hr/>			
RAW MATERIALS			
AMMONIA	8.75 ¢/LB	0.623722 LB	5.46
CAUSTIC SODA	11 ¢/LB	0.00373 LB	0.04
CYCLOHEXANE	15.62 ¢/LB	0.972984 LB	15.20
HYDROGEN	0.388 ¢/FT^3	0.01119 FT^3	NEGL
NYLON 6 SCARP	64.5 ¢/LB	0.06493 LB	4.19
OLEUM (7%)	4.01 ¢/LB	1.23005 LB	4.93
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
OTHER CHEMICALS	-- ¢/LB	-- LB	1.80
<hr/>			
GROSS RAW MATERIALS			31.83
<hr/>			
BY-PRODUCTS			
AMMONIUM SULFATE	1.9 ¢/LB	-1.685 LB	-3.20
FUEL	2.21 \$/MMBTU	-0.00095 MMBTU	-0.21
<hr/>			
TOTAL BY-PRODUCTS			-3.41

	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
<hr/>			
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	171 GAL	1,430 LITERS
PROCESS WATER	1.101 \$/MGAL	0.543 GAL	4.53 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	14.9 LB	14.9 KG
STEAM, 600 PSIG	5.72 \$/MLB	10.8 LB	10.8 KG
STEAM, 1500 PSIG	6.16 \$/MLB	3.88 LB	3.88 KG
ELECTRICITY	4 ¢/KWH	0.544 KWH	1.2 KWH
NATURAL GAS	3.24 \$/MMBTU	664 BTU	369 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.766 SCF	47.8 LITERS
REFRIGERATION, 40°F	5 ¢/TON-HR	0.176 TON-HR	1.36 KWH
<hr/>			
TOTAL UTILITIES			19.95

Table 7.3 (Concluded)
ECONOMICS OF N6-SBU2

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	77	154#	309
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	179.9	244.4	351.9
OFFSITES	98.2	151.4	244.7
TOTAL FIXED CAPITAL (TFC)	278.1	395.8	596.7
SCALING EXPONENTS	0.51	0.59	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	31.83	31.83	31.83
BY-PRODUCTS	-3.41	-3.41	-3.41
UTILITIES	19.95	19.95	19.95
VARIABLE COSTS	48.37	48.37	48.37
OPERATING LABOR, 19/SHIFT, \$33.58/HOUR	7.24	3.62	1.81
MAINTENANCE LABOR, 3%/YR OF BLI	6.99	4.75	3.42
CONTROL LAB LABOR, 20% OF OPER LABOR	1.45	0.72	0.36
LABOR COSTS	15.68	9.09	5.59
MAINTENANCE MATERIALS, 3%/YR OF BLI	6.99	4.75	3.42
OPERATING SUPPLIES, 10% OF OPER LABOR	0.72	0.36	0.18
TOTAL DIRECT COSTS	71.76	62.57	57.56
PLANT OVERHEAD, 80% OF LABOR COSTS	12.54	7.27	4.47
TAXES AND INSURANCE, 2%/YR OF TFC	7.21	5.13	3.87
PLANT CASH COSTS	91.51	74.97	65.90
DEPRECIATION, 10%/YR OF TFC	36.04	25.65	19.33
PLANT GATE COSTS	127.55	100.62	85.23
G&A, SALES, RESEARCH	12.00	12.00	12.00
NET PRODUCTION COST	139.55	112.62	97.23
ROI BEFORE TAXES, 25%/YR OF TFC	90.10	64.11	48.33
PRODUCT VALUE	229.65	176.73	145.56

* OF NYLON 6 CHIPS

BASE CASE

Table 7.4
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	\$/LB
RAW MATERIALS			
CAPROLACTAM	79.3 ¢/LB	0.94769 LB	75.15
NYLON 6 SCRAP	64.5 ¢/LB	0.06493 LB	4.19
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
CAUSTIC SODA	11 ¢/LB	0.00373 LB	0.04
OTHER CHEMICALS	-- ¢/LB	-- LB	0.02
GROSS RAW MATERIALS			79.61
UTILITIES			
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
COOLING WATER	7.45 ¢/MGAL	25.5 GAL	213 LITERS
PROCESS WATER	1.101 \$/MGAL	0.0343 GAL	0.287 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	1.07 LB	1.07 KG
STEAM, 600 PSIG	5.72 \$/MLB	1.17 LB	1.17 KG
STEAM, 1500 PSIG	6.16 \$/MLB	3.86 LB	3.86 KG
ELECTRICITY	4 ¢/KWH	0.145 KWH	0.321 KWH
NATURAL GAS	3.24 \$/MMBTU	250 BTU	139 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.143 SCF	8.93 LITERS
TOTAL UTILITIES			4.39

Table 7.4 (Concluded)
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	77	154#	309
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	40.1	56.2	83.1
OFFSITES	27.7	41.5	64.4
TOTAL FIXED CAPITAL (TFC)	67.8	97.7	147.5
SCALING EXPONENTS	0.53	0.59	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	79.61	79.61	79.61
UTILITIES	4.39	4.39	4.39
VARIABLE COSTS	84.00	84.00	84.00
OPERATING LABOR, 4/SHIFT, \$33.58/HR	1.52	0.76	0.38
MAINTENANCE LABOR, 3%/YR OF BLI	1.56	1.09	0.81
CONTROL LAB LABOR, 20% OF OPER LABOR	0.30	0.15	0.08
LABOR COSTS	3.38	2.00	1.27
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.56	1.09	0.81
OPERATING SUPPLIES, 10% OF OPER LABOR	0.15	0.08	0.04
TOTAL DIRECT COSTS	89.09	87.17	86.12
PLANT OVERHEAD, 80% OF LABOR COSTS	2.70	1.60	1.02
TAXES AND INSURANCE, 2%/YR OF TFC	1.76	1.27	0.96
PLANT CASH COSTS	93.55	90.04	88.10
DEPRECIATION, 10%/YR OF TFC	8.78	6.33	4.78
PLANT GATE COSTS	102.33	96.37	92.88
G&A, SALES, RESEARCH	12.00	12.00	12.00
NET PRODUCTION COST	114.33	108.37	104.88
ROI BEFORE TAXES, 25%/YR OF TFC	21.96	15.83	11.95
PRODUCT VALUE	136.29	124.20	116.83

* OF NYLON 6 CHIPS

BASE CASE

N6-SBU3 Description

The configuration of this SBU is determined with the status of DSM's CAPM and nylon 6 chips production in Western Europe in mind. The company has a 485 million lb/yr (220,000 t/yr) CAPM plant at Geleen, and Netherlands and an 187.4 million lb/yr (85,000 t/yr) nylon 6 resin plant at Emmen, Netherlands. The nylon 6 production in this case is at 187.4 million lb/yr (85,000 t/yr) and the CAPM production capacity is scaled down from the 485 million lb/yr (220,000 t/yr) to match the nylon production. The price of captive CAPM used in a stand-alone nylon 6 plant is derived from the 485 million lb/yr (220,000 t/yr) plant, which uses a phenol-based CAPM HPO process.

N6-SBU3 Cost Estimates

Table 7.5 presents the economics of N6-SBU3. The battery limits for the integrated unit is estimated at \$210.1 million and total fixed capital is \$340 million. With a unit price of phenol at 32 ¢/lb, the cash cost and the plant gate cost for nylon 6 are estimated at 73.6 ¢/lb and 92.5 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 151.7 ¢/lb.

In the present case, the price of captive CAPM produced by the 485 million lb/yr (220,000 t/yr) plant is estimated at 80.9 ¢/lb. The economics of a stand-alone nylon 6 plant of 187.4 million lb/yr (85,000 t/yr) with this CAPM price are then generated and given in Table 7.6. It appears that the product value for nylon 6 is reduced by nearly 19% to 123.4 ¢/lb when CAPM is captively derived from this large precursor plant.

N6-SBU4 Description

The CAPM used in this SBU is produced by a butadiene-based process jointly developed by DSM and DuPont as described in Section 6 of this report. The process produces CAPM via 6-aminocaproate. The configuration of this SBU is hypothetically assumed as same as N6-SBU1. Thus the nylon 6 production in this case is at 154.3 million lb/yr (70,000 t/yr) and the CAPM production capacity is scaled down from a 330 million lb/yr (150,000 t/yr) plant to match the nylon production. The price of captive CAPM used in a stand-alone nylon 6 plant is derived from the 330 million lb/yr (150,000 t/yr) plant using the butadiene-based CAPM process mentioned above.

N6-SBU4 Cost Estimates

Table 7.7 presents the economics of N6-SBU4. The battery limits for the integrated unit is estimated at \$210.1 million and total fixed capital is \$340 million. With a unit price of butadiene at 32 ¢/lb, the cash cost and the plant gate cost for nylon 6 are estimated at 53.6 ¢/lb and 75.7 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 142.7 ¢/lb.

In the present case, the price of captive CAPM produced by an assumed 330 million lb/yr (150,000 t/yr) plant is estimated at 63.1 ¢/lb. The economics of a stand-alone nylon 6 plant of 154.3 million lb/yr (70,000 t/yr) with this CAPM price are then generated and given in Table 7.8. It appears that the product value for nylon 6 is reduced by nearly 24% to 108.9 ¢/lb when CAPM is captively derived from this large precursor plant.

Table 7.5
ECONOMICS OF N6-SBU3

PRODUCTION COSTS

PEP COST INDEX: 624

VARIABLE COSTS

	UNIT COST	CONSUMPTION PER LB	\$/LB
<hr/>			
RAW MATERIALS			
AMMONIA	8.75 ¢/LB	0.623722 LB	5.46
CAUSTIC SODA	11 ¢/LB	0.00373 LB	0.04
PHENOL	32 ¢/LB	0.83643 LB	26.77
HYDROGEN	0.388 ¢/FT^3	0.0188 FT^3	0.01
NYLON 6 SCARP	64.5 ¢/LB	0.06493 LB	4.19
OLEUM (7%)	4.01 ¢/LB	1.23005 LB	4.93
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
OTHER CHEMICALS	-- ¢/LB	-- LB	1.95
<hr/>			
GROSS RAW MATERIALS			43.56
<hr/>			
BY-PRODUCTS			
AMMONIUM SULFATE	1.9 ¢/LB	-1.685 LB	-3.20
FUEL	2.21 \$/MMBTU	-0.00038 MMBTU	-0.08
<hr/>			
TOTAL BY-PRODUCTS			-3.28

	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG	
<hr/>				
UTILITIES				
COOLING WATER	7.45 ¢/MGAL	102 GAL	852 LITERS	0.76
PROCESS WATER	1.101 \$/MGAL	0.416 GAL	3.48 LITERS	0.05
STEAM, 150 PSIG	4.51 \$/MLB	13.7 LB	13.7 KG	6.19
STEAM, 600 PSIG	5.72 \$/MLB	1.3 LB	1.3 KG	0.75
STEAM, 1500 PSIG	6.16 \$/MLB	3.87 LB	3.87 KG	2.38
ELECTRICITY	4 ¢/KWH	0.422 KWH	0.93 KWH	1.69
NATURAL GAS	3.24 \$/MMBTU	294 BTU	164 KCAL	0.10
INERT GAS, LOW P	0.51 \$/MSCF	1.3 SCF	81.4 LITERS	0.07
REFRIGERATION, 40°F	5 ¢/TON-HR	0.176 TON-HR	1.36 KWH	0.88
<hr/>				
TOTAL UTILITIES				12.87

Table 7.5 (Concluded)
ECONOMICS OF N6-SBU3

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	94	187#	375
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	161.6	222.4	323.6
OFFSITES	87.8	131.4	210.7
-----	-----	-----	-----
TOTAL FIXED CAPITAL (TFC)	249.4	353.8	534.3
SCALING EXPONENTS	0.50	0.60	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	43.56	43.56	43.56
BY-PRODUCTS	-3.28	-3.28	-3.28
UTILITIES	12.87	12.87	12.87
-----	-----	-----	-----
VARIABLE COSTS	53.15	53.15	53.15
OPERATING LABOR, 19/SHIFT, \$33.58/HR	5.96	2.98	1.49
MAINTENANCE LABOR, 3%/YR OF BLI	5.17	3.56	2.59
CONTROL LAB LABOR, 20% OF OPER LABOR	1.19	0.60	0.30
-----	-----	-----	-----
LABOR COSTS	12.32	7.14	4.38
MAINTENANCE MATERIALS, 3%/YR OF BLI	5.17	3.56	2.59
OPERATING SUPPLIES, 10% OF OPER LABOR	0.60	0.30	0.15
-----	-----	-----	-----
TOTAL DIRECT COSTS	71.24	64.15	60.27
PLANT OVERHEAD, 80% OF LABOR COSTS	9.86	5.71	3.50
TAXES AND INSURANCE, 2%/YR OF TFC	5.32	3.78	2.85
-----	-----	-----	-----
PLANT CASH COSTS	86.42	73.64	66.62
DEPRECIATION, 10%/YR OF TFC	26.62	18.88	14.26
-----	-----	-----	-----
PLANT GATE COSTS	113.04	92.52	80.88
G&A, SALES, RESEARCH	12.00	12.00	12.00
-----	-----	-----	-----
NET PRODUCTION COST	125.04	104.52	92.88
ROI BEFORE TAXES, 25%/YR OF TFC	66.54	47.19	35.64
-----	-----	-----	-----
PRODUCT VALUE	191.58	151.71	128.52

* OF NYLON 6

BASE CASE

Table 7.6
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	\$/LB
RAW MATERIALS			
CAPROLACTAM	80.9 ¢/LB	0.94769 LB	76.67
NYLON 6 SCRAP	64.5 ¢/LB	0.06493 LB	4.19
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
CAUSTIC SODA	11 ¢/LB	0.00373 LB	0.04
OTHER CHEMICALS	-- ¢/LB	-- LB	0.02
GROSS RAW MATERIALS			81.13
UTILITIES			
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
COOLING WATER	7.45 ¢/MGAL	25.5 GAL	213 LITERS
PROCESS WATER	1.101 \$/MGAL	0.0343 GAL	0.287 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	1.07 LB	1.07 KG
STEAM, 600 PSIG	5.72 \$/MLB	1.17 LB	1.17 KG
STEAM, 1500 PSIG	6.16 \$/MLB	3.86 LB	3.86 KG
ELECTRICITY	4 ¢/KWH	0.144 KWH	0.319 KWH
NATURAL GAS	3.24 \$/MMBTU	250 BTU	139 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.143 SCF	8.93 LITERS
TOTAL UTILITIES			4.39

Table 7.6 (Concluded)
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	94	187 [#]	375
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	44.1	62.5	93.3
OFFSITES	31.0	46.9	73.2
TOTAL FIXED CAPITAL (TFC)	75.1	109.4	166.4
SCALING EXPONENTS	0.54	0.60	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	81.13	81.13	81.13
UTILITIES	4.39	4.39	4.39
VARIABLE COSTS	85.52	85.52	85.52
OPERATING LABOR, 4/SHIFT, \$33.58/HR	1.26	0.63	0.31
MAINTENANCE LABOR, 3%/YR OF BLI	1.41	1.00	0.75
CONTROL LAB LABOR, 20% OF OPER LABOR	0.25	0.13	0.06
LABOR COSTS	2.92	1.76	1.12
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.41	1.00	0.75
OPERATING SUPPLIES, 10% OF OPER LABOR	0.13	0.06	0.03
TOTAL DIRECT COSTS	89.98	88.34	87.42
PLANT OVERHEAD, 80% OF LABOR COSTS	2.34	1.41	0.90
TAXES AND INSURANCE, 2%/YR OF TFC	1.60	1.17	0.89
PLANT CASH COSTS	93.92	90.92	89.21
DEPRECIATION, 10%/YR OF TFC	8.02	5.84	4.44
PLANT GATE COSTS	101.94	96.76	93.65
G&A, SALES, RESEARCH	12.00	12.00	12.00
NET PRODUCTION COST	113.94	108.76	105.65
ROI BEFORE TAXES, 25%/YR OF TFC	20.04	14.60	11.10
PRODUCT VALUE	133.98	123.36	116.75

* OF NYLON 6 CHIPS

BASE CASE

Table 7.7
ECONOMICS OF N6-SBU4

PRODUCTION COSTS

PEP COST INDEX: 624

VARIABLE COSTS

	UNIT COST	CONSUMPTION PER LB	\$/LB
<hr/>			
RAW MATERIALS			
AMMONIA	8.75 ¢/LB	0.142135 LB	1.24
BUTADIENE	11 ¢/LB	0.53081 LB	5.84
CAUSTIC SODA	11 ¢/FT^3	0.00373 FT^3	0.04
CARBON MONOXIDE	0.24 ¢/FT^3	0.006792 FT^3	NEGL
HYDROGEN	0.388 ¢/FT^3	0.006309 FT^3	NEGL
METHANOL	6.82 ¢/LB	0.04667 LB	0.32
NYLON 6 SCRAP	64.5 ¢/LB	0.06493 LB	4.19
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
OTHER CHEMICALS	-- ¢/LB	-- LB	0.02
<hr/>			
GROSS RAW MATERIALS			11.86

	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG	
<hr/>				
UTILITIES				
COOLING WATER	7.45 ¢/MGAL	164 GAL	1,370 LITERS	1.22
PROCESS WATER	1.101 \$/MGAL	0.0337 GAL	0.281 LITERS	NEGL
STEAM, 150 PSIG	4.51 \$/MLB	20.3 LB	20.3 KG	9.17
STEAM, 600 PSIG	5.72 \$/MLB	1.18 LB	1.18 KG	0.67
STEAM, 1500 PSIG	6.16 \$/MLB	9.76 LB	9.76 KG	6.01
ELECTRICITY	4 ¢/KWH	0.422 KWH	0.93 KWH	1.69
NATURAL GAS	3.24 \$/MMBTU	255 BTU	142 KCAL	0.08
INERT GAS, LOW P	0.51 \$/MSCF	0.307 SCF	19.1 LITERS	0.02
REFRIGERATION, 40°F	5.01 ¢/TON-HR	0.0405 TON-HR	0.314 KWH	0.20
<hr/>				
TOTAL UTILITIES				19.06

Table 7.7 (Concluded)
ECONOMICS OF N6-SBU4

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	77	154#	309
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	150.3	210.1	318.2
OFFSITES	85.6	129.9	214.3
TOTAL FIXED CAPITAL (TFC)	235.9	340.0	532.5
SCALING EXPONENTS	0.53	0.65	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	11.86	11.86	11.86
UTILITIES	19.06	19.06	19.06
VARIABLE COSTS	30.92	30.92	30.92
OPERATING LABOR, 16/SHIFT, \$33.58/HR	6.10	3.05	1.52
MAINTENANCE LABOR, 3%/YR OF BLI	5.84	4.08	3.09
CONTROL LAB LABOR, 20% OF OPER LABOR	1.22	0.61	0.30
LABOR COSTS	13.16	7.74	4.91
MAINTENANCE MATERIALS, 3%/YR OF BLI	5.84	4.08	3.09
OPERATING SUPPLIES, 10% OF OPER LABOR	0.61	0.30	0.15
TOTAL DIRECT COSTS	50.53	43.04	39.07
PLANT OVERHEAD, 80% OF LABOR COSTS	10.53	6.19	3.93
TAXES AND INSURANCE, 2%/YR OF TFC	6.11	4.41	3.45
PLANT CASH COSTS	67.17	53.64	46.45
DEPRECIATION, 10%/YR OF TFC	30.57	22.03	17.25
PLANT GATE COSTS	97.74	75.67	63.70
G&A, SALES, RESEARCH	12.00	12.00	12.00
NET PRODUCTION COST	109.74	87.67	75.70
ROI BEFORE TAXES, 25%/YR OF TFC	76.43	55.07	43.14
PRODUCT VALUE	186.17	142.74	118.84

* OF NYLON 6

BASE CASE

Table 7.8
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	\$/LB
RAW MATERIALS			
CAPROLACTAM	63.1 ¢/LB	0.94769 LB	59.80
NYLON 6 SCRAP	64.5 ¢/LB	0.06493 LB	4.19
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
CAUSTIC SODA	11 ¢/LB	0.00373 LB	0.04
OTHER CHEMICALS	-- ¢/LB	-- LB	0.02
GROSS RAW MATERIALS			64.26
UTILITIES			
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
COOLING WATER	7.45 ¢/MGAL	25.5 GAL	213 LITERS
PROCESS WATER	1.101 \$/MGAL	0.0343 GAL	0.287 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	1.07 LB	1.07 KG
STEAM, 600 PSIG	5.72 \$/MLB	1.17 LB	1.17 KG
STEAM, 1500 PSIG	6.16 \$/MLB	3.86 LB	3.86 KG
ELECTRICITY	4 ¢/KWH	0.145 KWH	0.321 KWH
NATURAL GAS	3.24 \$/MMBTU	250 BTU	139 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.143 SCF	8.93 LITERS
TOTAL UTILITIES			4.39

Table 7.8 (Concluded)
CONTINUOUS PRODUCTION OF NYLON 6 CHIPS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	77	154#	309
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	40.1	56.2	83.1
OFFSITES	27.7	41.5	64.4
TOTAL FIXED CAPITAL (TFC)	67.8	97.7	147.5
SCALING EXPONENTS	0.53	0.59	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	64.26	64.26	64.26
UTILITIES	4.39	4.39	4.39
VARIABLE COSTS	68.65	68.65	68.65
OPERATING LABOR, 4/SHIFT, \$33.58/HR	1.52	0.76	0.38
MAINTENANCE LABOR, 3%/YR OF BLI	1.56	1.09	0.81
CONTROL LAB LABOR, 20% OF OPER LABOR	0.30	0.15	0.08
LABOR COSTS	3.38	2.00	1.27
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.56	1.09	0.81
OPERATING SUPPLIES, 10% OF OPER LABOR	0.15	0.08	0.04
TOTAL DIRECT COSTS	73.74	71.82	70.77
PLANT OVERHEAD, 80% OF LABOR COSTS	2.70	1.60	1.02
TAXES AND INSURANCE, 2%/YR OF TFC	1.76	1.27	0.96
PLANT CASH COSTS	78.20	74.69	72.75
DEPRECIATION, 10%/YR OF TFC	8.78	6.33	4.78
PLANT GATE COSTS	86.98	81.02	77.53
G&A, SALES, RESEARCH	12.00	12.00	12.00
NET PRODUCTION COST	98.98	93.02	89.53
ROI BEFORE TAXES, 25%/YR OF TFC	21.96	15.83	11.95
PRODUCT VALUE	120.94	108.85	101.48

* OF NYLON 6 CHIPS

BASE CASE

N6-SBU5 Description

The CAPM used in this SBU is produced by an ADN-based process, which produces CAPM and HMDA at equal amounts. The process is jointly developed by BASF and DuPont as described in Section 6 of this report. We integrated this process with a butadiene-based ADN process using hydrocyanation technology at a design capacity of 330 million lb/yr (150,000 t/yr). The configuration of this SBU is then assumed to combine a nylon 6 production at 165.3 million lb/yr (75,000 t/yr) and a CAPM production from the integrated butadiene-based CAPM/HMDA process. Two alternative cases are considered:

- Case A – The Nylon 6 production is combined with the CAPM production by integrating half of the capital investment, and raw material and utilities consumption from the CAPM-HMDA plant to those of the nylon 6 plant. In such a case, the co-product HMDA is not credited.
- Case B – The Nylon 6 production is combined with the CAPM production by integrating total of the capital investment, and raw material and utilities consumption from the CAPM-HMDA plant to those of the nylon 6 plant. In such a case, the co-product HMDA is credited.

N6-SBU5 Cost Estimates

Table 7.9 presents the economics of Case A of the N6-SBU5. The battery limits for the integrated unit is estimated at \$152.2 million and total fixed capital is \$337.4 million. With a unit price of butadiene at 13 ¢/lb, the cash cost and the plant gate cost for nylon 6 are estimated at 84.3 ¢/lb and 104.7 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 167.7 ¢/lb.

Table 7.10 gives the economics of Case B of the N6-SBU5 with HMDA credited as a co-product. The battery limits, in this case, is estimated at \$248.9 million and total fixed capital is \$563.8 million. With a unit price of butadiene at 13 ¢/lb and HMDA is credited at 110 ¢/lb, the plant cash cost and the plant gate cost for nylon 6 are reduced to 45.2 ¢/lb and 31.5 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 170.5 ¢/lb.

Table 7.9
ECONOMICS OF N6-SBU5--CASE A

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
AMMONIA	8.75 ¢/LB	0.001725 LB	0.02
BUTADIENE	13 ¢/LB	0.535975 LB	6.97
CAUSTIC SODA	11 ¢/LB	0.00373 LB	0.04
CYCLOHEXANE	15.62 ¢/LB	0.000578 LB	0.01
ETHANOL	155 ¢/GALLON	0.001194 GALLON	0.19
HYDROGEN	0.388 ¢/FT^3	0.009494 FT^3	NEGL
HYDROGEN CYANIDE	46.18 ¢/LB	0.533795 LB	24.65
NYLON 6 SCRAP	64.5 ¢/LB	0.06493 LB	4.19
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
PHOSPHORUS TRICHLORIDE	49 ¢/LB	0.003374 LB	0.17
SODIUM BISULFITE	19.25 ¢/LB	0.108151 LB	2.08
SODIUM SULFITE	30.5 ¢/LB	0.065647 LB	2.00
TRIPHENYLBORANE	10.26 \$/LB	0.000123 LB	0.13
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.00019 LB	0.05
OTHER CHEMICALS	-- ¢/LB	-- LB	0.02
GROSS RAW MATERIALS			40.73
UTILITIES			
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
COOLING WATER	7.45 ¢/MGAL	121 GAL	1,010 LITERS
PROCESS WATER	1.101 \$/MGAL	0.421 GAL	3.51 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	5.82 LB	5.82 KG
STEAM, 600 PSIG	5.72 \$/MLB	16.1 LB	16.1 KG
STEAM, 1500 PSIG	6.16 \$/MLB	13.4 LB	13.4 KG
ELECTRICITY	4 ¢/KWH	0.247 KWH	0.544 KWH
NATURAL GAS	3.24 \$/MMBTU	405 BTU	225 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.405 SCF	25.3 LITERS
REFRIGERATION, 20°F	5.09 ¢/TON-HR	0.57 TON-HR	4.42 KWH
REFRIGERATION, 40°F	5 ¢/TON-HR	0.0439 TON-HR	0.341 KWH
TOTAL UTILITIES			25.28

Table 7.9 (Concluded)
ECONOMICS OF N6-SBU5--CASE A

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	83	165#	331
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	107.9	152.2	227.2
OFFSITES	109.0	185.2	325.9
-----	-----	-----	-----
TOTAL FIXED CAPITAL (TFC)	217.0	337.4	553.1
SCALING EXPONENTS	0.64	0.71	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	40.73	40.73	40.73
UTILITIES	25.28	25.28	25.28
-----	-----	-----	-----
VARIABLE COSTS	66.01	66.01	66.01
OPERATING LABOR, 16/SHIFT, \$33.58/HOUR	5.69	2.85	1.42
MAINTENANCE LABOR, 3%/YR OF BLI	3.92	2.76	2.06
CONTROL LAB LABOR, 20% OF OPER LABOR	1.14	0.57	0.28
-----	-----	-----	-----
LABOR COSTS	10.75	6.18	3.76
MAINTENANCE MATERIALS, 3%/YR OF BLI	3.92	2.76	2.06
OPERATING SUPPLIES, 10% OF OPER LABOR	0.57	0.28	0.14
-----	-----	-----	-----
TOTAL DIRECT COSTS	81.25	75.23	71.97
PLANT OVERHEAD, 80% OF LABOR COSTS	8.60	4.94	3.01
TAXES AND INSURANCE, 2%/YR OF TFC	5.25	4.08	3.35
-----	-----	-----	-----
PLANT CASH COSTS	95.10	84.25	78.33
DEPRECIATION, 10%/YR OF TFC	26.25	20.41	16.73
-----	-----	-----	-----
PLANT GATE COSTS	121.35	104.66	95.06
G&A, SALES, RESEARCH	12.00	12.00	12.00
-----	-----	-----	-----
NET PRODUCTION COST	133.35	116.66	107.06
ROI BEFORE TAXES, 25%/YR OF TFC	65.63	51.03	41.83
-----	-----	-----	-----
PRODUCT VALUE	198.98	167.69	148.89

* OF NYLON 66

BASE CASE

Table 7.10
ECONOMICS of N6-SBU5—CASE B

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
AMMONIA	8.75 ¢/LB	0.00345 LB	0.03
BUTADIENE	13 ¢/LB	1.07195 LB	13.94
CAUSTIC SODA	11 ¢/LB	0.00373 LB	0.04
CYCLOHEXANE	15.62 ¢/LB	0.001156 LB	0.02
ETHANOL	155 ¢/GALLON	0.002388 GALLON	0.37
HYDROGEN	0.388 ¢/FT^3	0.018988 FT^3	0.01
HYDROGEN CYANIDE	46.18 ¢/LB	1.06759 LB	49.30
NYLON 6 SCRAP	64.5 ¢/LB	0.06493 LB	4.19
PHOSPHORIC ACID	34 ¢/LB	0.00616 LB	0.21
PHOSPHORUS TRICHLORIDE	49 ¢/LB	0.006747 LB	0.33
SODIUM BISULFITE	19.25 ¢/LB	0.216301 LB	4.16
SODIUM SULFITE	30.5 ¢/LB	0.131293 LB	4.00
TRIPHENYLBORANE	10.26 \$/LB	0.000246 LB	0.25
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.000379 LB	0.11
OTHER CHEMICALS	-- ¢/LB	-- LB	0.02
GROSS RAW MATERIALS			76.98
BY-PRODUCTS			
HMDA	110 ¢/LB	-1 LB	-110.00
TOTAL BY-PRODUCTS			-110.00
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	216 GAL	1,800 LITERS
PROCESS WATER	1.101 \$/MGAL	0.807 GAL	6.74 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	10.6 LB	10.6 KG
STEAM, 600 PSIG	5.72 \$/MLB	31 LB	31 KG
STEAM, 1500 PSIG	6.16 \$/MLB	22.9 LB	22.9 KG
ELECTRICITY	4 ¢/KWH	0.349 KWH	0.769 KWH
NATURAL GAS	3.24 \$/MMBTU	572 BTU	318 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	0.668 SCF	41.7 LITERS
REFRIGERATION, 20°F	5.08 ¢/TON-HR	1.14 TON-HR	8.84 KWH
REFRIGERATION, 40°F	5 ¢/TON-HR	0.0879 TON-HR	0.681 KWH
TOTAL UTILITIES			46.18

**Table 7.10 (Concluded)
ECONOMICS OF N6-SBU5—CASE B**

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	83	165#	331
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	176.4	248.9	372.6
OFFSITES	182.5	315.0	558.5
TOTAL FIXED CAPITAL (TFC)	359.0	563.8	931.1
SCALING EXPONENTS	0.65	0.72	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	76.98	76.98	76.98
BY-PRODUCTS	-110.00	-110.00	-110.00
UTILITIES	46.18	46.18	46.18
VARIABLE COSTS	13.16	13.16	13.16
OPERATING LABOR, 16/SHIFT, \$33.58/HR	5.69	2.85	1.42
MAINTENANCE LABOR, 3%/YR OF BLI	6.40	4.52	3.38
CONTROL LAB LABOR, 20% OF OPER LABOR	1.14	0.57	0.28
LABOR COSTS	13.23	7.94	5.08
MAINTENANCE MATERIALS, 3%/YR OF BLI	6.40	4.52	3.38
OPERATING SUPPLIES, 10% OF OPER LABOR	0.57	0.28	0.14
TOTAL DIRECT COSTS	33.36	25.90	21.76
PLANT OVERHEAD, 80% OF LABOR COSTS	10.58	6.35	4.06
TAXES AND INSURANCE, 2%/YR OF TFC	8.69	6.82	5.63
PLANT CASH COSTS	52.63	39.07	31.45
DEPRECIATION, 10%/YR OF TFC	43.43	34.11	28.16
PLANT GATE COSTS	96.06	73.18	59.61
G&A, SALES, RESEARCH	12.00	12.00	12.00
NET PRODUCTION COST	108.06	85.18	71.61
ROI BEFORE TAXES, 25%/YR OF TFC	108.58	85.28	70.41
PRODUCT VALUE	216.64	170.46	142.02

* OF NYLON 66

BASE CASE

STRATEGIC UNITS FOR THE PRODUCTION OF NYLON 66 RESINS

N66-SBU1 Description

The configuration of this SBU is determined with the status of DuPont's ADA, HMDA and nylon 66 resins production in the United States in mind. DuPont has its largest ADA plant at Victoria, TX with a production capacity of 835 million lb/yr (379,000 t/yr). The plant uses cyclohexane-based oxidation process for ADA. The company's largest HMDA plant is located at Orange, TX with a production capacity of 730 million lb/yr (331,000 t/yr). The Victoria plant uses butadiene-based hydrocyanation process for HMDA. The company has nylon 66 resin production at various locations around the world. The largest plant at Parkersburg, WV has a production capacity of 176 million lb/yr (80,000 t/yr). We select the Parkersburg plant as the production base for N66-SBU1. The production capacities of ADA and HMDA are scaled down respectively from the two precursor plants mentioned above to match the nylon production. Alternatively, we estimate the net production costs of ADA and HMDA from the above precursor plants, which are used for the captive precursors employed in a stand-alone nylon 66 resin plant.

N66-SBU1 Cost Estimates

Table 7.11 presents the economics of N66-SBU1. The battery limits for the integrated unit is estimated at \$222.4 million and total fixed capital is \$335.7 million. With unit prices of cyclohexane and butadiene at 15.62 ¢/lb and 13 ¢/lb respectively, the cash cost and the plant gate cost for nylon 66 resin are estimated at about 68 ¢/lb and 87 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 149.6 ¢/lb.

Table 7.12 presents the economics for the stand-alone resin plant using captive ADA HMDA from the two precursor plants. We estimate the net production cost for ADA at 43.8 ¢/lb, and that for HMDA at 66.7 ¢/lb. In such a case, the product value for nylon 66 resin is reduced by about 32% to 101.9 ¢/lb.

N66-SBU2 Description

The configuration of this SBU is hypothetically defined with a butadiene-based carboalkoxylation process for ADA, which is integrated with similar HMDA and nylon 66 processes as used in N66-SBU1. The nylon 66 production capacity in this case is also 176 million lb/yr (80,000 t/yr) with the production capacities of ADA and HMDA hypothetically scaled down respectively from a 835 million lb/yr (379,000 t/yr) plant and a 730 million lb/yr (331,000 t/yr) plant to matched the nylon production. In an alternative case, the prices of captive ADA and HMDA used in a stand-alone nylon 66 plant are also derived from the large precursor plants.

N66-SBU2 Cost Estimates

Table 7.13 presents the economics of N66-SBU2. The battery limits for the integrated unit is estimated at \$219.4 million and total fixed capital is \$331.0 million. With unit price of butadiene at 13 ¢/lb, the cash cost and the plant gate cost for nylon 66 resin are estimated at about 59.7 ¢/lb and 78.5 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 140.4 ¢/lb.

Table 7.14 summarizes the economics for the stand-alone nylon 66 resin plant with captive ADA and HMDA. The unit price for ADA is estimated at 39.9 ¢/lb, and that for HMDA at 66.7 ¢/lb. As indicated in this table, the product value for nylon 66 resin is reduced by 29% to 99.4 ¢/lb.

Table 7.11
ECONOMICS OF N66-SBU1

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05
AMMONIA	8.75 ¢/LB	0.000858 LB	0.01
AMMONIUM VANADATE	86 ¢/LB	0.000039 LB	NEGL
BUTADIENE	13 ¢/LB	0.28166 LB	3.66
CARBON DIOXIDE	3.24 ¢/LB	0.000858 LB	NEGL
CAUSTIC SODA	11 ¢/LB	0.03227 LB	0.35
COBALT NAPHTHENATE	3.71 \$/LB	0.000485 LB	0.18
CUPRIC NITRATE	1.3 \$/LB	0.000091 LB	0.01
CYCLOHEXANE	15.62 ¢/LB	0.47232 LB	7.38
HYDROGEN	0.388 ¢/FT^3	0.006498 FT^3	NEGL
HYDROGEN CYANIDE	46.18 ¢/FT^3	0.28052 FT^3	12.95
IRON CATALYST	1.1 \$/LB	0.0031 LB	0.34
NICKEL POWDER	8.5 \$/LB	0.0002 LB	0.17
NITRIC ACID	18.3 ¢/LB	0.384399 LB	7.03
PHOSPHOROUS TRICHLORIDE	49 ¢/LB	0.0001 LB	NEGL
SODIUM BISULFITE	19.25 ¢/LB	0.056833 LB	1.09
SODIUM SULFITE	30.5 ¢/LB	0.034497 LB	1.05
SULFURIC ACID	2.3 ¢/LB	0.054038 LB	0.12
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.001773 LB	0.49
TRIPHENYLBORANE	10.26 \$/LB	0.000062 LB	0.06
GROSS RAW MATERIALS			34.94
BY-PRODUCTS			
DIBASIC ACIDS	12.9 ¢/LB	-0.08758 LB	-1.13
HEXAMETHYLENEIMINE	2.21 \$/LB	-0.00207 LB	-0.46
HEAVY AMINE	35 ¢/LB	-0.00672 LB	-0.24
TOTAL BY-PRODUCTS			-1.83
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	73.7 GAL	615 LITERS
PROCESS WATER	1.101 \$/MGAL	0.177 GAL	1.48 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	11.6 LB	11.6 KG
STEAM, 600 PSIG	5.72 \$/MLB	4.29 LB	4.29 KG
ELECTRICITY	4 ¢/KWH	0.276 KWH	0.609 KWH
NATURAL GAS	3.24 \$/MMBTU	44.7 BTU	24.8 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	1.47 SCF	92.1 LITERS
REFRIGERATION, 40°F	5.04 ¢/TON-HR	0.0145 TON-HR	0.113 KWH
TOTAL UTILITIES			9.51

Table 7.11 (Concluded)
ECONOMICS OF N66-SBU1

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	88	176#	353
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	163.6	222.4	318.7
OFFSITES	77.4	113.3	174.5
-----	-----	-----	-----
TOTAL FIXED CAPITAL (TFC)	241.0	335.7	493.1
SCALING EXPONENTS	0.48	0.55	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	34.94	34.94	34.94
BY-PRODUCTS	-1.83	-1.83	-1.83
UTILITIES	9.51	9.51	9.51
-----	-----	-----	-----
VARIABLE COSTS	42.62	42.62	42.62
OPERATING LABOR, 29/SHIFT, \$33.58/HR	9.67	4.84	2.42
MAINTENANCE LABOR, 3%/YR OF BLI	5.56	3.78	2.71
CONTROL LAB LABOR, 20% OF OPER LABOR	1.93	0.97	0.48
-----	-----	-----	-----
LABOR COSTS	17.16	9.59	5.61
MAINTENANCE MATERIALS, 3%/YR OF BLI	5.56	3.78	2.71
OPERATING SUPPLIES, 10% OF OPER LABOR	0.97	0.48	0.24
-----	-----	-----	-----
TOTAL DIRECT COSTS	66.31	56.47	51.18
PLANT OVERHEAD, 80% OF LABOR COSTS	13.73	7.67	4.49
TAXES AND INSURANCE, 2%/YR OF TFC	5.46	3.81	2.80
-----	-----	-----	-----
PLANT CASH COSTS	85.50	67.95	58.47
DEPRECIATION, 10%/YR OF TFC	27.32	19.03	13.98
-----	-----	-----	-----
PLANT GATE COSTS	112.82	86.98	72.45
G&A, SALES, RESEARCH	15.00	15.00	15.00
-----	-----	-----	-----
NET PRODUCTION COST	127.82	101.98	87.45
ROI BEFORE TAXES, 25%/YR OF TFC	68.31	47.57	34.94
-----	-----	-----	-----
PRODUCT VALUE	196.13	149.55	122.39

* OF NYLON 66 RESIN

BASE CASE

Table 7.12
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
ADIPIC ACID	43.8 ¢/LB	0.646538 LB	28.32
HEXAMETHYLENE DIAMINE	66.7 ¢/LB	0.517043 LB	34.49
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05
GROSS RAW MATERIALS			62.86
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	8.42 GAL	70.3 LITERS
PROCESS WATER	1.101 \$/MGAL	0.0946 GAL	0.79 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	2.68 LB	2.68 KG
ELECTRICITY	4 ¢/KWH	0.135 KWH	0.297 KWH
INERT GAS, LOW P	0.51 \$/MSCF	1.1 SCF	68.9 LITERS
TOTAL UTILITIES			1.88

Table 7.12 (Concluded)
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	88	176#	353
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	39.0	55.6	83.1
OFFSITES	19.3	28.6	43.7
TOTAL FIXED CAPITAL (TFC)	58.3	84.2	126.7
SCALING EXPONENTS	0.53	0.59	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	62.86	62.86	62.86
UTILITIES	1.88	1.88	1.88
VARIABLE COSTS	64.74	64.74	64.74
OPERATING LABOR, 5/SHIFT, \$33.58/HR	1.67	0.83	0.42
MAINTENANCE LABOR, 3%/YR OF BLI	1.33	0.95	0.71
CONTROL LAB LABOR, 20% OF OPER LABOR	0.33	0.17	0.08
LABOR COSTS	3.33	1.95	1.21
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.33	0.95	0.71
OPERATING SUPPLIES, 10% OF OPER LABOR	0.17	0.08	0.04
TOTAL DIRECT COSTS	69.57	67.72	66.70
PLANT OVERHEAD, 80% OF LABOR COSTS	2.66	1.56	0.97
TAXES AND INSURANCE, 2%/YR OF TFC	1.32	0.95	0.72
PLANT CASH COSTS	73.55	70.23	68.39
DEPRECIATION, 10%/YR OF TFC	6.61	4.77	3.59
PLANT GATE COSTS	80.16	75.00	71.98
G&A, SALES, RESEARCH	15.00	15.00	15.00
NET PRODUCTION COST	95.16	90.00	86.98
ROI BEFORE TAXES, 25%/YR OF TFC	16.51	11.93	8.98
PRODUCT VALUE	111.67	101.93	95.96

* OF NYLON 66 RESIN

BASE CASE

Table 7.13
ECONOMICS OF N66-SBU2

PRODUCTION COSTS

PEP COST INDEX: 624

VARIABLE COSTS

	UNIT COST	CONSUMPTION PER LB	\$/LB
<hr/>			
RAW MATERIALS			
ACETIC ACID	31 ¢/LB	0.004316 LB	0.13
AMMONIA	8.75 ¢/LB	0.000858 LB	0.01
MIXED C4 FEED	11.74 ¢/LB	0.780688 LB	9.17
BUTADIENE	13 ¢/LB	0.28166 LB	3.66
CARBON DIOXIDE	3.24 ¢/LB	0.000858 LB	NEGL
CARBON MONOXIDE	0.898 ¢/FT^3	0.20333 FT^3	0.18
COBALT ACETATE	9.78 \$/LB	0.000194 LB	0.19
CYCLOHEXANE	15.62 ¢/LB	0.00031 LB	NEGL
HYDROGEN	0.388 ¢/FT^3	0.011103 FT^3	NEGL
HYDROGEN CYANIDE	46.18 ¢/FT^3	0.28052 FT^3	12.95
IRON CATALYST	1.1 \$/LB	0.0031 LB	0.34
NICKEL POWDER	8.5 \$/LB	0.0002 LB	0.17
METHANOL	6.82 ¢/LB	0.01757 LB	0.12
PHOSPHOROUS TRICHLORIDE	49 ¢/LB	0.000103 LB	0.01
POTASSIUM SULFATE	100 ¢/LB	0.000129 LB	0.01
PYRIDINE	3.878 \$/LB	0.002108 LB	0.82
SODIUM BISULFITE	19.25 ¢/LB	0.056833 LB	1.09
SODIUM SULFITE	30.5 ¢/LB	0.034497 LB	1.05
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.001773 LB	0.49
TRIPHENYLBORANE	10.26 \$/LB	0.000062 LB	0.06
<hr/>			
GROSS RAW MATERIALS			30.45
<hr/>			
BY-PRODUCTS			
DIBASIC ACIDS	12.9 ¢/LB	-0.14126 LB	-1.82
HEXAMETHYLENEIMINE	2.21 \$/LB	-0.002068 LB	-0.46
HEAVY AMINE	35 ¢/LB	-0.006722 LB	-0.24
MIXED C4 BY-PRODUCTS	4 ¢/LB	-0.44054 LB	-1.76
METHYL VALERATE	38 ¢/LB	-0.02931 LB	-1.11
<hr/>			
TOTAL BY-PRODUCTS			-5.39

	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG	
<hr/>				
UTILITIES				
COOLING WATER	7.45 ¢/MGAL	73.7 GAL	615 LITERS	0.55
PROCESS WATER	1.101 \$/MGAL	0.177 GAL	1.48 LITERS	0.02
STEAM, 150 PSIG	4.51 \$/MLB	11.6 LB	11.6 KG	5.22
STEAM, 600 PSIG	5.72 \$/MLB	4.29 LB	4.29 KG	2.45
ELECTRICITY	4 ¢/KWH	0.276 KWH	0.609 KWH	1.11
NATURAL GAS	3.24 \$/MMBTU	44.7 BTU	24.8 KCAL	0.01
INERT GAS, LOW P	0.51 \$/MSCF	1.47 SCF	92.1 LITERS	0.08
REFRIGERATION, 40°F	5.04 ¢/TON-HR	0.0145 TON-HR	0.113 KWH	0.07
<hr/>				
TOTAL UTILITIES				9.51

Table 7.13 (Concluded)
ECONOMICS OF N66-SBU2

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	88	176#	353
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	155.6	219.4	330.0
OFFSITES	74.0	111.6	177.6
-----	-----	-----	-----
TOTAL FIXED CAPITAL (TFC)	229.6	331.0	507.6
SCALING EXPONENTS	0.53	0.62	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	30.45	30.45	30.45
BY-PRODUCTS	-5.39	-5.39	-5.39
UTILITIES	9.51	9.51	9.51
-----	-----	-----	-----
VARIABLE COSTS	34.57	34.57	34.57
OPERATING LABOR, 29/SHIFT, \$33.58/HR	9.67	4.84	2.42
MAINTENANCE LABOR, 3%/YR OF BLI	5.29	3.73	2.81
CONTROL LAB LABOR, 20% OF OPER LABOR	1.93	0.97	0.48
-----	-----	-----	-----
LABOR COSTS	16.89	9.54	5.71
MAINTENANCE MATERIALS, 3%/YR OF BLI	5.29	3.73	2.81
OPERATING SUPPLIES, 10% OF OPER LABOR	0.97	0.48	0.24
-----	-----	-----	-----
TOTAL DIRECT COSTS	57.72	48.32	43.33
PLANT OVERHEAD, 80% OF LABOR COSTS	13.51	7.63	4.57
TAXES AND INSURANCE, 2%/YR OF TFC	5.21	3.75	2.88
-----	-----	-----	-----
PLANT CASH COSTS	76.44	59.70	50.78
DEPRECIATION, 10%/YR OF TFC	26.03	18.76	14.39
-----	-----	-----	-----
PLANT GATE COSTS	102.47	78.46	65.17
G&A, SALES, RESEARCH	15.00	15.00	15.00
-----	-----	-----	-----
NET PRODUCTION COST	117.47	93.46	80.17
ROI BEFORE TAXES, 25%/YR OF TFC	65.08	46.91	35.97
-----	-----	-----	-----
PRODUCT VALUE	182.55	140.37	116.14

* OF NYLON 66 RESIN

BASE CASE

Table 7.14
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
ADIPIC ACID	39.9 ¢/LB	0.646538 LB	25.80
HEXAMETHYLENE DIAMINE	66.7 ¢/LB	0.517043 LB	34.49
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05
GROSS RAW MATERIALS			60.34
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	8.42 GAL	70.3 LITERS
PROCESS WATER	1.101 \$/MGAL	0.0946 GAL	0.79 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	2.68 LB	2.68 KG
ELECTRICITY	4 ¢/KWH	0.135 KWH	0.297 KWH
INERT GAS, LOW P	0.51 \$/MSCF	1.1 SCF	68.9 LITERS
TOTAL UTILITIES			1.88

Table 7.14 (Concluded)
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	88	176#	353
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	39.0	55.6	83.1
OFFSITES	19.3	28.6	43.7
TOTAL FIXED CAPITAL (TFC)	58.3	84.2	126.7
SCALING EXPONENTS	0.53	0.59	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	60.34	60.34	60.34
UTILITIES	1.88	1.88	1.88
VARIABLE COSTS	62.22	62.22	62.22
OPERATING LABOR, 5/SHIFT, \$33.58/HR	1.67	0.83	0.42
MAINTENANCE LABOR, 3%/YR OF BLI	1.33	0.95	0.71
CONTROL LAB LABOR, 20% OF OPER LABOR	0.33	0.17	0.08
LABOR COSTS	3.33	1.95	1.21
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.33	0.95	0.71
OPERATING SUPPLIES, 10% OF OPER LABOR	0.17	0.08	0.04
TOTAL DIRECT COSTS	67.05	65.20	64.18
PLANT OVERHEAD, 80% OF LABOR COSTS	2.66	1.56	0.97
TAXES AND INSURANCE, 2%/YR OF TFC	1.32	0.95	0.72
PLANT CASH COSTS	71.03	67.71	65.87
DEPRECIATION, 10%/YR OF TFC	6.61	4.77	3.59
PLANT GATE COSTS	77.64	72.48	69.46
G&A, SALES, RESEARCH	15.00	15.00	15.00
NET PRODUCTION COST	92.64	87.48	84.46
ROI BEFORE TAXES, 25%/YR OF TFC	16.51	11.93	8.98
PRODUCT VALUE	109.15	99.41	93.44

* OF NYLON 66 RESIN

BASE CASE

N66-SBU3 Description

The configuration of this SBU is determined with the status of Asahi Chemical's ADA, HMDA and nylon 66 resins production in Japan in mind. Asahi has its ADA plant at Nobeoka, Miyazaki Prefecture with a production capacity of 264.6 million lb/yr (120,000 t/yr). The plant uses benzene as raw material, which is partial hydrogenate and hydrated to cyclohexanol. The latter is subjected to oxidation process to produce ADA. Also at Nobeoka, the company has a 94.8 million lb/yr (43,000 t/yr) HMDA plant using butadiene-based hydrocyanation process, and a 99.2 million lb/yr (45,000 t/yr) nylon 66 resin plant. We select the Nobeoka resin plant as the production base for N66-SBU3. The production capacities of ADA and HMDA are scaled down respectively from the two precursor plants mentioned above to match the nylon production. Alternatively, we estimate the net production costs of ADA and HMDA from the above precursor plants, which are used for the captive precursors employed in a stand-alone nylon 66 resin plant.

N66-SBU3 Cost Estimates

Table 7.15 presents the economics of N66-SBU1. The battery limits for the integrated unit is estimated at \$181 million and total fixed capital is \$270.5 million. With unit prices of benzene and butadiene at 9.5 ¢/lb and 13 ¢/lb respectively, the cash cost and the plant gate cost for nylon 66 resin are estimated at about 77.2 ¢/lb and 104.5 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 187.7 ¢/lb.

Table 7.16 presents the economics for the stand-alone resin plant using captive ADA HMDA from the two precursor plants. We estimate the net production cost for ADA at 55.4 ¢/lb, and that for HMDA at 84.5 ¢/lb. In such a case, the product value for nylon 66 resin is reduced by nearly 33% to 126 ¢/lb.

N66-SBU4 Description

The configuration of this SBU is determined with the status of DuPont's ADA, HMDA and nylon 66 resins production in the United States in mind. DuPont has its largest ADA plant at Victoria, TX with a production capacity of 835 million lb/yr (379,000 t/yr). The plant uses cyclohexane-based oxidation process for ADA. The company's largest HMDA plant is located at Orange, TX with a production capacity of 730 million lb/yr (331,000 t/yr). The Victoria plant uses butadiene-based hydrocyanation process for HMDA. The company has nylon 66 resin production at various locations around the world. The largest plant at Parkersburg, WV has a production capacity of 176 million lb/yr (80,000 t/yr). We select the Parkersburg plant as the production base for N66-SBU1. The production capacities of ADA and HMDA are scaled down respectively from the two precursor plants mentioned above to match the nylon production. Alternatively, we estimate the net production costs of ADA and HMDA from the above precursor plants, which are used for the captive precursors employed in a stand-alone nylon 66 resin plant.

N66-SBU4 Cost Estimates

Table 7.17 presents the economics of N66-SBU4. The battery limits for the integrated unit is estimated at \$195.4 million and total fixed capital is \$297.2 million. With unit prices of cyclohexane and butadiene at 15.62 ¢/lb and 13 ¢/lb respectively, the cash cost and the plant gate cost for nylon 66 resin are estimated at about 57.6 ¢/lb and 71.8 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 122.3 ¢/lb.

Table 7.18 presents the economics for the stand-alone resin plant using captive ADA HMDA from the two precursor plants. We estimate the net production cost for ADA at 43.9 ¢/lb, and that for HMDA at 58.6 ¢/lb. In such a case, the product value for nylon 66 resin is reduced by about 24% to 93.1 ¢/lb.

N66-SBU5 Description

The HMDA used in this SBU is produced by an ADN-based process, which produces CAPM and HMDA at equal amounts. The process is jointly developed by BASF and DuPont as described in Section 6 of this report. We integrated this process with a butadiene-based ADN process using hydrocyanation technology at a design capacity of 330 million lb/yr (150,000 t/yr). The configuration of this SBU is assumed to combine a nylon 66 production at 298 million lb/yr (135,000 t/yr) with a HMDA production from the integrated butadiene-based CAPM/HMDA process and an ADA production of 192 million lb/yr (87,300 t/yr), using a cyclohexane-based oxidation process. Two alternative cases are considered:

- Case A – The nylon 66 production is combined with the ADA production and HMDA production by integrating half of the capital investment, and raw material and utilities consumption from the CAPM-HMDA plant to those of the nylon 66 process and the ADA process. In such a case, the co-product CAPM is not credited.
- Case B – The Nylon 66 production is combined with the ADA production and HMDA production by integrating total of the capital investment, and raw material and utilities consumption from the CAPM-HMDA plant to those of the nylon 66 process and the ADA process. In such a case, the co-product CAPM is credited.

N66-SBU5 Cost Estimates

Table 7.19 presents the economics of Case A of the N66-SBU5. The battery limits for the integrated unit is estimated at \$260.4 million and total fixed capital is \$494.1 million. With a unit price of butadiene at 13 ¢/lb, the cash cost and the plant gate cost for nylon 6 are estimated at 76.5 ¢/lb and 93.1 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 149.6 ¢/lb.

Table 7.20 gives the economics of Case B of the N66-SBU5 with CAPM credited as a co-product. The battery limits, in this case, is estimated at \$356.5 million and total fixed capital is \$722.3 million. With a unit price of butadiene at 13 ¢/lb and CAPM is credited at 90 ¢/lb, the plant cash cost and the plant gate cost for nylon 66 are reduced to 22.7 ¢/lb and 46.9 ¢/lb respectively. After addition of costs for G&A, sales and research, and 25% pretax annual return on total fixed capital, the product value for the resin is estimated at 122.6 ¢/lb.

Table 7.15
ECONOMICS OF N66-SBU3

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	\$/LB
RAW MATERIALS			
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05
AMMONIA	8.75 ¢/LB	0.000858 LB	0.01
BENZENE	9.5 ¢/LB	0.51062 LB	4.85
BUTADIENE	13 ¢/LB	0.28166 LB	3.66
CARBON DIOXIDE	3.24 ¢/LB	0.000858 LB	NEGL
CUPRIC NITRATE	1.3 \$/FT^3	0.000091 FT^3	0.01
CYCLOHEXANE	15.62 ¢/LB	0.00031 LB	NEGL
HYDROGEN	0.388 ¢/FT^3	0.011635 FT^3	NEGL
HYDROGEN CYANIDE	46.18 ¢/FT^3	0.28052 FT^3	12.95
IRON CATALYST	1.1 \$/LB	0.0031 LB	0.34
NICKEL POWDER	8.5 \$/LB	0.0002 LB	0.17
NITRIC ACID	18.3 ¢/LB	0.3844 LB	7.03
PHOSPHOROUS TRICHLORIDE	49 ¢/LB	0.000103 LB	0.01
ADIPONITRILE	42 ¢/LB	0.000052 LB	NEGL
AMMONIUM VANADATE	86 ¢/LB	0.000039 LB	NEGL
SODIUM BISULFITE	19.25 ¢/LB	0.056833 LB	1.09
SODIUM SULFITE	30.5 ¢/LB	0.034497 LB	1.05
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.001773 LB	0.49
TRIPHENYLBORANE	10.26 \$/LB	0.000062 LB	0.06
CYCLOHEXANE	15.3 ¢/LB	0.000305 LB	NEGL
RU/ZN CATALYST	8.66 \$/LB	0.000084 LB	0.07
ZEM CATALYST	2.4 \$/LB	0.000886 LB	0.21
GROSS RAW MATERIALS			32.05
BY-PRODUCTS			
CYCLOHEXANE	14.7 ¢/LB	-0.11445 LB	-1.68
HEXAMETHYLENEIMINE	2.21 \$/LB	-0.002068 LB	-0.46
HEAVY AMINE	35 ¢/LB	-0.006722 LB	-0.24
MIXED DIBASIC ACIDS	12.9 ¢/LB	-0.03774 LB	-0.49
TOTAL BY-PRODUCTS			-2.87
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	75.2 GAL	627 LITERS
PROCESS WATER	1.101 \$/MGAL	0.194 GAL	1.62 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	11 LB	11 KG
STEAM, 600 PSIG	5.72 \$/MLB	6.44 LB	6.44 KG
ELECTRICITY	4 ¢/KWH	0.422 KWH	0.93 KWH
NATURAL GAS	3.24 \$/MMBTU	44.7 BTU	24.8 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	1.33 SCF	83.1 LITERS
REFRIGERATION, 20°F	5.14 ¢/TON-HR	0.0323 TON-HR	0.25 KWH
REFRIGERATION, 40°F	5.08 ¢/TON-HR	0.0126 TON-HR	0.098 KWH
TOTAL UTILITIES			11.21

Table 7.15 (Concluded)
ECONOMICS OF N66-SBU3

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	50	99#	198
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	139.2	181.0	245.1
OFFSITES	64.1	89.6	133.4
-----	-----	-----	-----
TOTAL FIXED CAPITAL (TFC)	203.4	270.5	378.5
SCALING EXPONENTS	0.41	0.48	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	32.05	32.05	32.05
BY-PRODUCTS	-2.87	-2.87	-2.87
UTILITIES	11.21	11.21	11.21
-----	-----	-----	-----
VARIABLE COSTS	40.39	40.39	40.39
OPERATING LABOR, 24/SHIFT, \$33.58/HR	14.23	7.12	3.56
MAINTENANCE LABOR, 3%/YR OF BLI	8.42	5.47	3.71
CONTROL LAB LABOR, 20% OF OPER LABOR	2.85	1.42	0.71
-----	-----	-----	-----
LABOR COSTS	25.50	14.01	7.98
MAINTENANCE MATERIALS, 3%/YR OF BLI	8.42	5.47	3.71
OPERATING SUPPLIES, 10% OF OPER LABOR	1.42	0.71	0.36
-----	-----	-----	-----
TOTAL DIRECT COSTS	75.73	60.58	52.44
PLANT OVERHEAD, 80% OF LABOR COSTS	20.40	11.21	6.38
TAXES AND INSURANCE, 2%/YR OF TFC	8.20	5.45	3.82
-----	-----	-----	-----
PLANT CASH COSTS	104.33	77.24	62.64
DEPRECIATION, 10%/YR OF TFC	41.01	27.27	19.08
-----	-----	-----	-----
PLANT GATE COSTS	145.34	104.51	81.72
G&A, SALES, RESEARCH	15.00	15.00	15.00
-----	-----	-----	-----
NET PRODUCTION COST	160.34	119.51	96.72
ROI BEFORE TAXES, 25%/YR OF TFC	102.51	68.18	47.70
-----	-----	-----	-----
PRODUCT VALUE	262.85	187.69	144.42

* OF NYLON 66 RESIN

BASE CASE

Table 7.16
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
ADIPIC ACID	55.4 ¢/LB	0.646538 LB	35.82
HEXAMETHYLENE DIAMINE	84.5 ¢/LB	0.517043 LB	43.69
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05
GROSS RAW MATERIALS			79.56
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	8.42 GAL	0.06
PROCESS WATER	1.101 \$/MGAL	0.0946 GAL	0.01
STEAM, 150 PSIG	4.51 \$/MLB	2.68 LB	2.68 KG
ELECTRICITY	4 ¢/KWH	0.139 KWH	0.305 KWH
INERT GAS, LOW P	0.51 \$/MSCF	1.1 SCF	68.9 LITERS
TOTAL UTILITIES			1.89

Table 7.16 (Concluded)
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	50	99#	198
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	29.2	40.7	59.3
OFFSITES	14.0	20.3	30.5
TOTAL FIXED CAPITAL (TFC)	43.2	61.0	89.8
SCALING EXPONENTS	0.50	0.56	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	79.56	79.56	79.56
UTILITIES	1.89	1.89	1.89
VARIABLE COSTS	81.45	81.45	81.45
OPERATING LABOR, 5/SHIFT, \$33.58/HR	2.97	1.48	0.74
MAINTENANCE LABOR, 3%/YR OF BLI	1.76	1.23	0.90
CONTROL LAB LABOR, 20% OF OPER LABOR	0.59	0.30	0.15
LABOR COSTS	5.32	3.01	1.79
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.76	1.23	0.90
OPERATING SUPPLIES, 10% OF OPER LABOR	0.30	0.15	0.07
TOTAL DIRECT COSTS	88.83	85.84	84.21
PLANT OVERHEAD, 80% OF LABOR COSTS	4.26	2.41	1.43
TAXES AND INSURANCE, 2%/YR OF TFC	1.74	1.23	0.91
PLANT CASH COSTS	94.83	89.48	86.55
DEPRECIATION, 10%/YR OF TFC	8.71	6.15	4.53
PLANT GATE COSTS	103.54	95.63	91.08
G&A, SALES, RESEARCH	15.00	15.00	15.00
NET PRODUCTION COST	118.54	110.63	106.08
ROI BEFORE TAXES, 25%/YR OF TFC	21.76	15.37	11.32
PRODUCT VALUE	140.30	126.00	117.40

* OF NYLON 66 RESIN

BASE CASE

Table 7.17
ECONOMICS OF N66-SBU4

PRODUCTION COSTS

PEP COST INDEX: 624

VARIABLE COSTS

	UNIT COST	CONSUMPTION PER LB	\$/LB
RAW MATERIALS			
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05
AMMONIA	8.75 ¢/LB	0.000858 LB	0.01
AMMONIUM VANADATE	86 ¢/LB	0.000039 LB	NEGL
BUTADIENE	13 ¢/LB	0.28166 LB	3.66
CARBON DIOXIDE	3.24 ¢/LB	0.000858 LB	NEGL
CAUSTIC SODA	11 ¢/LB	0.03227 LB	0.35
COBALT NAPHTHENATE	3.71 \$/LB	0.000485 LB	0.18
CUPRIC NITRATE	1.3 \$/LB	0.000091 LB	0.01
CYCLOHEXANE	15.62 ¢/LB	0.47232 LB	7.38
HYDROGEN	0.388 ¢/FT ³	0.006498 FT ³	NEGL
HYDROGEN CYANIDE	46.18 ¢/FT ³	0.28052 FT ³	12.95
IRON CATALYST	1.1 \$/LB	0.0031 LB	0.34
NICKEL POWDER	8.5 \$/LB	0.0002 LB	0.17
NITRIC ACID	18.3 ¢/LB	0.384399 LB	7.03
PHOSPHOROUS TRICHLORIDE	49 ¢/LB	0.0001 LB	NEGL
SODIUM BISULFITE	19.25 ¢/LB	0.056833 LB	1.09
SODIUM SULFITE	30.5 ¢/LB	0.034497 LB	1.05
SULFURIC ACID	2.3 ¢/LB	0.054038 LB	0.12
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.001773 LB	0.49
TRIPHENYLBORANE	10.26 \$/LB	0.000062 LB	0.06
GROSS RAW MATERIALS			34.94
BY-PRODUCTS			
DIBASIC ACIDS	12.9 ¢/LB	-0.08758 LB	-1.13
HEXAMETHYLENEIMINE	2.21 \$/LB	-0.00207 LB	-0.46
HEAVY AMINE	35 ¢/LB	-0.00672 LB	-0.24
TOTAL BY-PRODUCTS			-1.83

	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG	
UTILITIES				
COOLING WATER	7.45 ¢/MGAL	59.5 GAL	496 LITERS	0.44
PROCESS WATER	1.101 \$/MGAL	0.0949 GAL	0.792 LITERS	0.01
STEAM, 150 PSIG	4.51 \$/MLB	10.2 LB	10.2 KG	4.58
STEAM, 600 PSIG	5.72 \$/MLB	2.97 LB	2.97 KG	1.70
ELECTRICITY	4 ¢/KWH	0.241 KWH	0.53 KWH	0.96
INERT GAS, LOW P	0.51 \$/MSCF	1.36 SCF	84.6 LITERS	0.07
REFRIGERATION, 40°F	5.21 ¢/TON-HR	0.00226 TON-HR	0.0175 KWH	0.01
TOTAL UTILITIES				7.77

Table 7.17 (Concluded)
ECONOMICS OF N66-SBU4

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	105	209#	419
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	140.5	195.4	283.5
OFFSITES	68.5	101.8	158.2
TOTAL FIXED CAPITAL (TFC)	209.0	297.2	441.7
SCALING EXPONENTS	0.51	0.57	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	34.94	34.94	34.94
BY-PRODUCTS	-1.83	-1.83	-1.83
UTILITIES	7.77	7.77	7.77
VARIABLE COSTS	40.88	40.88	40.88
OPERATING LABOR, 19/SHIFT, \$33.58/HR	5.34	2.67	1.33
MAINTENANCE LABOR, 3%/YR OF BLI	4.03	2.80	2.03
CONTROL LAB LABOR, 20% OF OPER LABOR	1.07	0.53	0.27
LABOR COSTS	10.44	6.00	3.63
MAINTENANCE MATERIALS, 3%/YR OF BLI	4.03	2.80	2.03
OPERATING SUPPLIES, 10% OF OPER LABOR	0.53	0.27	0.13
TOTAL DIRECT COSTS	55.88	49.95	46.67
PLANT OVERHEAD, 80% OF LABOR COSTS	8.35	4.80	2.90
TAXES AND INSURANCE, 2%/YR OF TFC	3.99	2.84	2.11
PLANT CASH COSTS	68.22	57.59	51.68
DEPRECIATION, 10%/YR OF TFC	19.96	14.19	10.55
PLANT GATE COSTS	88.18	71.78	62.23
G&A, SALES, RESEARCH	15.00	15.00	15.00
NET PRODUCTION COST	103.18	86.78	77.23
ROI BEFORE TAXES, 25%/YR OF TFC	49.91	35.48	26.37
PRODUCT VALUE	153.09	122.26	103.60

* OF NYLON 66 RESIN

BASE CASE

Table 7.18
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	¢/LB
RAW MATERIALS			
ADIPIC ACID	43.9 ¢/LB	0.646538 LB	28.38
HEXAMETHYLENE DIAMINE	58.6 ¢/LB	0.517043 LB	30.30
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05
GROSS RAW MATERIALS			58.73
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	8.42 GAL	0.06
PROCESS WATER	1.101 \$/MGAL	0.0946 GAL	0.01
STEAM, 150 PSIG	4.51 \$/MLB	2.68 LB	2.68 KG
ELECTRICITY	4 ¢/KWH	0.134 KWH	0.295 KWH
INERT GAS, LOW P	0.51 \$/MSCF	1.1 SCF	68.9 LITERS
TOTAL UTILITIES			1.88

Table 7.18 (Concluded)
NYLON 66 RESIN BY CONTINUOUS PROCESS

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	105	209#	419
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	42.8	61.2	91.5
OFFSITES	21.2	31.5	48.4
TOTAL FIXED CAPITAL (TFC)	64.0	92.7	139.9
SCALING EXPONENTS	0.53	0.59	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	58.73	58.73	58.73
UTILITIES	1.88	1.88	1.88
VARIABLE COSTS	60.61	60.61	60.61
OPERATING LABOR, 5/SHIFT, \$33.58/HR	1.40	0.70	0.35
MAINTENANCE LABOR, 3%/YR OF BLI	1.23	0.88	0.66
CONTROL LAB LABOR, 20% OF OPER LABOR	0.28	0.14	0.07
LABOR COSTS	2.91	1.72	1.08
MAINTENANCE MATERIALS, 3%/YR OF BLI	1.23	0.88	0.66
OPERATING SUPPLIES, 10% OF OPER LABOR	0.14	0.07	0.04
TOTAL DIRECT COSTS	64.89	63.28	62.39
PLANT OVERHEAD, 80% OF LABOR COSTS	2.33	1.38	0.86
TAXES AND INSURANCE, 2%/YR OF TFC	1.22	0.89	0.67
PLANT CASH COSTS	68.44	65.55	63.92
DEPRECIATION, 10%/YR OF TFC	6.11	4.43	3.34
PLANT GATE COSTS	74.55	69.98	67.26
G&A, SALES, RESEARCH	12.00	12.00	12.00
NET PRODUCTION COST	86.55	81.98	79.26
ROI BEFORE TAXES, 25%/YR OF TFC	15.28	11.07	8.35
PRODUCT VALUE	101.83	93.05	87.61

* OF NYLON 66 RESIN

BASE CASE

Table 7.19
ECONOMICS OF N66-SBU5--CASE A

PRODUCTION COSTS				
PEP COST INDEX: 624				
VARIABLE COSTS				
	UNIT COST	CONSUMPTION PER LB	\$/LB	
RAW MATERIALS				
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05	
AMMONIA	8.75 ¢/LB	0.000941 LB	0.01	
AMMONIUM VANADATE	86 ¢/LB	0.000039 LB	NEGL	
BUTADIENE	13 ¢/LB	0.292419 LB	3.80	
CAUSTIC SODA	11 ¢/LB	0.032269 LB	0.35	
COBALT NAPHTHENATE	3.71 \$/LB	0.000485 LB	0.18	
CUPRIC NITRATE	1.3 \$/LB	0.000091 LB	0.01	
CYCLOHEXANE	15.62 ¢/LB	0.730365 LB	11.41	
ETHANOL	155 ¢/GALLON	0.000652 GALLON	0.10	
HYDROGEN	0.388 ¢/FT^3	0.005179 FT^3	NEGL	
HYDROGEN CYANIDE	46.18 ¢/LB	0.291229 LB	13.45	
NICKEL POWDER	8.79 \$/LB	0.000212 LB	0.19	
NITRIC ACID	18.3 ¢/LB	0.387987 LB	7.10	
PHOSPHORUS TRICHLORIDE	49 ¢/LB	0.000105 LB	0.01	
SODIUM BISULFITE	19.25 ¢/LB	0.059017 LB	1.14	
SODIUM SULFITE	30.5 ¢/LB	0.035823 LB	1.09	
SULFURIC ACID	2.3 ¢/LB	0.54542 LB	1.25	
TRIPHENYLBORANE	10.26 \$/LB	0.000067 LB	0.07	
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.001841 LB	0.51	
MIXED DIBASIC ACIDS	12.9 ¢/LB	0.088397 LB	1.14	
GROSS RAW MATERIALS			41.86	
BY-PRODUCTS				
LIGHT ENDS AS FUEL	2.21 \$/MMBTU	-0.000341 MMBTU	-0.08	
TOTAL BY-PRODUCTS			-0.08	
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG	
UTILITIES				
COOLING WATER	7.45 ¢/MGAL	97.9 GAL	817 LITERS	0.73
PROCESS WATER	1.101 \$/MGAL	0.31 GAL	2.59 LITERS	0.03
STEAM, 150 PSIG	4.51 \$/MLB	12.6 LB	12.6 KG	5.69
STEAM, 600 PSIG	5.72 \$/MLB	8.97 LB	8.97 KG	5.13
STEAM, 1500 PSIG	6.16 \$/MLB	5.29 LB	5.29 KG	3.26
ELECTRICITY	4 ¢/KWH	0.227 KWH	0.5 KWH	0.91
NATURAL GAS	3.24 \$/MMBTU	92.7 BTU	51.5 KCAL	0.03
INERT GAS, LOW P	0.51 \$/MSCF	1.39 SCF	86.8 LITERS	0.07
REFRIGERATION, 20°F	5.09 ¢/TON-HR	0.316 TON-HR	2.45 KWH	1.61
REFRIGERATION, 40°F	5.02 ¢/TON-HR	0.0267 TON-HR	0.207 KWH	0.13
TOTAL UTILITIES			17.59	

Table 7.19 (Concluded)
ECONOMICS OF N66-SBU5--CASE A

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	149	298#	595
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	187.8	260.4	378.3
OFFSITES	143.4	233.7	399.5
TOTAL FIXED CAPITAL (TFC)	331.2	494.1	777.8
SCALING EXPONENTS	0.58	0.65	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	41.86	41.86	41.86
BY-PRODUCTS	-0.08	-0.08	-0.08
UTILITIES	17.59	17.59	17.59
VARIABLE COSTS	59.37	59.37	59.37
OPERATING LABOR, 29/SHIFT, \$33.58/HOUR	5.73	2.87	1.43
MAINTENANCE LABOR, 3%/YR OF BLI	3.79	2.62	1.91
CONTROL LAB LABOR, 20% OF OPER LABOR	1.15	0.57	0.29
LABOR COSTS	10.67	6.06	3.63
MAINTENANCE MATERIALS, 3%/YR OF BLI	3.79	2.62	1.91
OPERATING SUPPLIES, 10% OF OPER LABOR	0.57	0.29	0.14
TOTAL DIRECT COSTS	74.40	68.34	65.05
PLANT OVERHEAD, 80% OF LABOR COSTS	8.54	4.85	2.90
TAXES AND INSURANCE, 2%/YR OF TFC	4.45	3.32	2.61
PLANT CASH COSTS	87.39	76.51	70.56
DEPRECIATION, 10%/YR OF TFC	22.25	16.60	13.07
PLANT GATE COSTS	109.64	93.11	83.63
G&A, SALES, RESEARCH	15.00	15.00	15.00
NET PRODUCTION COST	124.64	108.11	98.63
ROI BEFORE TAXES, 25%/YR OF TFC	55.64	41.51	32.67
PRODUCT VALUE	180.28	149.62	131.30

* OF NYLON 66

BASE CASE

Table 7.20
ECONOMICS OF N66-SBU5--CASE B

PRODUCTION COSTS			
PEP COST INDEX: 624			
VARIABLE COSTS			
	UNIT COST	CONSUMPTION PER LB	\$/LB
RAW MATERIALS			
ACETIC ACID	31 ¢/LB	0.00173 LB	0.05
AMMONIA	8.75 ¢/LB	0.001882 LB	0.02
AMMONIUM VANADATE	86 ¢/LB	0.000039 LB	NEGL
BUTADIENE	13 ¢/LB	0.584838 LB	7.60
CAUSTIC SODA	11 ¢/LB	0.032269 LB	0.35
COBALT NAPHTHENATE	3.71 \$/LB	0.000485 LB	0.18
CUPRIC NITRATE	1.3 \$/LB	0.000091 LB	0.01
CYCLOHEXANE	15.62 ¢/LB	0.730681 LB	11.41
ETHANOL	155 ¢/GALLON	0.001303 GALLON	0.20
HYDROGEN	0.388 ¢/FT^3	0.010359 FT^3	NEGL
HYDROGEN CYANIDE	46.18 ¢/LB	0.582459 LB	26.90
NICKEL POWDER	8.79 \$/LB	0.000424 LB	0.37
NITRIC ACID	18.3 ¢/LB	0.387987 LB	7.10
PHOSPHORUS TRICHLORIDE	49 ¢/LB	0.00021 LB	0.01
SODIUM BISULFITE	19.25 ¢/LB	0.118034 LB	2.27
SODIUM SULFITE	30.5 ¢/LB	0.071646 LB	2.19
SULFURIC ACID	2.3 ¢/LB	0.54542 LB	1.25
TRIPHENYLBORANE	10.26 \$/LB	0.000134 LB	0.14
TRI-O-TOLYLPHOSPHITE	2.79 \$/LB	0.003682 LB	1.03
MIXED DIBASIC ACIDS	12.9 ¢/LB	0.088397 LB	1.14
GROSS RAW MATERIALS			62.22
BY-PRODUCTS			
LIGHT ENDS AS FUEL	2.21 \$/MMBTU	-0.000683 MMBTU	-0.15
CAPM	90 ¢/LB	-1 LB	-90.00
TOTAL BY-PRODUCTS			-90.15
	UNIT COST	CONSUMPTION PER LB	CONSUMPTION PER KG
UTILITIES			
COOLING WATER	7.45 ¢/MGAL	151 GAL	1,260 LITERS
PROCESS WATER	1.101 \$/MGAL	0.525 GAL	4.38 LITERS
STEAM, 150 PSIG	4.51 \$/MLB	15.3 LB	15.3 KG
STEAM, 600 PSIG	5.72 \$/MLB	17.3 LB	17.3 KG
STEAM, 1500 PSIG	6.16 \$/MLB	10.6 LB	10.6 KG
ELECTRICITY	4 ¢/KWH	0.283 KWH	0.624 KWH
NATURAL GAS	3.24 \$/MMBTU	185 BTU	103 KCAL
INERT GAS, LOW P	0.51 \$/MSCF	1.54 SCF	95.9 LITERS
REFRIGERATION, 20°F	5.08 ¢/TON-HR	0.633 TON-HR	4.91 KWH
REFRIGERATION, 40°F	5 ¢/TON-HR	0.051 TON-HR	0.396 KWH
TOTAL UTILITIES			29.20

Table 7.20 (Concluded)
ECONOMICS OF N66-SBU5--CASE B

PRODUCTION COSTS			
PEP COST INDEX: 624			
CAPACITY (MILLION LB/YR)*	149	298#	595
INVESTMENT (\$ MILLIONS)	-----	-----	-----
BATTERY LIMITS (BLI)	255.8	356.5	522.9
OFFSITES	217.6	365.8	638.2
TOTAL FIXED CAPITAL (TFC)	473.4	722.3	1161.2
SCALING EXPONENTS	0.61	0.68	
PRODUCTION COSTS (\$/LB)			
RAW MATERIALS	62.22	62.22	62.22
BY-PRODUCTS	-90.15	-90.15	-90.15
UTILITIES	29.20	29.20	29.20
VARIABLE COSTS	1.27	1.27	1.27
OPERATING LABOR, 29/SHIFT, \$33.58/HR	5.73	2.87	1.43
MAINTENANCE LABOR, 3%/YR OF BLI	5.16	3.59	2.64
CONTROL LAB LABOR, 20% OF OPER LABOR	1.15	0.57	0.29
LABOR COSTS	12.04	7.03	4.36
MAINTENANCE MATERIALS, 3%/YR OF BLI	5.16	3.59	2.64
OPERATING SUPPLIES, 10% OF OPER LABOR	0.57	0.29	0.14
TOTAL DIRECT COSTS	19.04	12.18	8.41
PLANT OVERHEAD, 80% OF LABOR COSTS	9.63	5.62	3.49
TAXES AND INSURANCE, 2%/YR OF TFC	6.36	4.85	3.90
PLANT CASH COSTS	35.03	22.65	15.80
DEPRECIATION, 10%/YR OF TFC	31.81	24.27	19.51
PLANT GATE COSTS	66.84	46.92	35.31
G&A, SALES, RESEARCH	15.00	15.00	15.00
NET PRODUCTION COST	81.84	61.92	50.31
ROI BEFORE TAXES, 25%/YR OF TFC	79.53	60.68	48.77
PRODUCT VALUE	161.37	122.60	99.08

* OF NYLON 66

BASE CASE

ECONOMICS COMPARISON OF SBUS FOR NYLON 6 AND NYLON 66 RESINS

Table 7.21 summarizes the economics of SBUs for nylon 6 resins. Also listed in the table are economics for a stand-alone nylon 6 resin plant under each of N6-SBU1 through N6-SBU4. In the case of N6-SBU5, two alternate cases, Case A and Case B, are presented. Similarly, those SBUs for nylon 66 resins are given in Table 7.22. Among the N6-SBUs, N6-SBU4 provides the best economics both at the integrated plant and stand-alone nylon 6 resin plant. The economics for N6-SBU5 is less than desirable in both Case A and Case B. Among the remaining three SBUs, their economics for the stand-alone nylon 6 plants are compatible within 6 % difference in product value. In the case of the integrated plant, the economics for N6-SBU2 is less favorable.

Table 7.22 summarizes the economics of SBUs for nylon 66 resins. Also listed in the table are economics for a stand-alone nylon 6 resin plant under each of N66-SBU1 through N66-SBU4. Two alternate cases, Case A and Case B, are also presented in the table. The economics for N66-SBU3 is less than desirable in both the integrated plant and the stand-alone nylon 66 resin plant. The size of the resin plant could be the major reason. The economics for the remaining for SBUs are compatible both at the integrated plant and the stand-alone plant with N66-SBU2 and N66-SBU4 more economically favorable.

Table 7.21
ECONOMICS OF SBUs FOR NYLON 6 RESINS

ECONOMIC COMPARISON					
CAPACITY: 300 MILLION LB/YR (136,000 T/YR)					
PEP COST INDEX: 624					
	N6-SBU1	N6-SBU2	N6-SBU3	N6-SBU4	N6-SBU5 Case A
PRODUCTION CAPACITY, MILLION LB/YR (THOUSAND METRIC TON/YR)	154	154	187	154	165
	(70)	(70)	(85)	(70)	(75)
INVESTMENT (\$ MILLIONS)					
BATTERY LIMITS (BLI)	200.2	244.4	222.4	210.1	152.2
OFFSITES	<u>131.7</u>	<u>151.4</u>	<u>131.4</u>	<u>129.9</u>	<u>185.2</u>
TOTAL FIXED CAPITAL (TFC)	331.9	395.8	353.8	340.0	337.4
PRODUCTION COSTS (\$/LB)					
RAW MATERIALS	31.31	31.83	43.56	11.86	40.73
BY-PRODUCTS	-3.46	-3.41	-3.28	--	--
UTILITIES	<u>17.42</u>	<u>19.95</u>	<u>12.87</u>	<u>19.06</u>	<u>25.28</u>
VARIABLE COSTS	45.27	48.37	53.15	30.92	66.01
LABOR COSTS	7.55	9.09	7.14	7.74	6.18
DIRECT COSTS	4.19	5.11	3.86	4.38	3.04
PLANT OVERHEAD, TAXES & INSURANCE	<u>10.34</u>	<u>12.40</u>	<u>9.49</u>	<u>10.60</u>	<u>9.02</u>
PLANT CASH COSTS	67.35	74.97	73.64	53.64	84.25
DEPRECIATION, 10%/YR OF TFC	<u>21.51</u>	<u>25.65</u>	<u>18.88</u>	<u>22.03</u>	<u>20.41</u>
PLANT GATE COSTS	88.86	100.62	92.52	75.67	104.66
G&A, SALES, RESEARCH	<u>12.00</u>	<u>12.00</u>	<u>12.00</u>	<u>12.00</u>	<u>12.00</u>
NET PRODUCTION COST	100.86	112.62	104.52	87.67	116.66
ROI BEFORE TAXES, 25%/YR OF TFC	<u>53.77</u>	<u>64.11</u>	<u>47.19</u>	<u>55.07</u>	<u>51.03</u>
PRODUCT VALUE	154.63	176.73	151.71	142.74	167.69

ECONOMICS FOR STAND-ALONE NYLON 6 PLANT WITH CAPTIVE PRECURSOR

	N6-SBU1	N6-SBU2	N6-SBU3	N6-SBU4	N6-SBU5 Case B
INVESTMENT (\$ MILLIONS)					
BATTERY LIMITS (BLI)	56.2	56.2	62.5	56.2	248.9
OFFSITES	<u>41.5</u>	<u>41.5</u>	<u>46.9</u>	<u>41.5</u>	<u>315.0</u>
TOTAL FIXED CAPITAL (TFC)	97.7	97.7	109.4	97.7	563.8
PRODUCTION COSTS (\$/LB)					
RAW MATERIALS	72.22	79.61	81.13	64.26	76.98
BY-PRODUCTS	--	--	--	--	-110.00
UTILITIES	<u>4.39</u>	<u>4.39</u>	<u>4.39</u>	<u>4.39</u>	<u>46.18</u>
VARIABLE COSTS	76.61	84.00	85.52	68.65	13.16
LABOR & OTHER FIXED COSTS	<u>6.04</u>	<u>6.04</u>	<u>2.82</u>	<u>6.04</u>	<u>12.74</u>
PLANT CASH COSTS	82.65	90.04	88.34	74.69	39.07
PLANT GATE COSTS	88.98	96.37	96.76	81.02	73.18
NET PRODUCTION COSTS	100.98	108.37	108.76	93.02	85.18
PRODUCT VALUE	116.81	124.20	123.36	108.85	170.46

Table 7.22
ECONOMICS OF SBUs FOR NYLON 66 RESINS

ECONOMIC COMPARISON

CAPACITY: 300 MILLION LB/YR (136,000 T/YR)

PEP COST INDEX: 624

	N66-SBU1	N66-SBU2	N66-SBU3	N66-SBU4	N66-SBU5 Case A
PRODUCTION CAPACITY, MILLION LB/YR (THOUSAND METRIC TON/YR)	176 (80)	176 (80)	99 (45)	209 (95)	298 (135)
INVESTMENT (\$ MILLIONS)					
BATTERY LIMITS (BLI)	222.4	219.4	181.0	195.4	260.4
OFFSITES	<u>113.3</u>	<u>111.6</u>	<u>89.6</u>	<u>101.8</u>	<u>233.7</u>
TOTAL FIXED CAPITAL (TFC)	335.7	331.0	270.5	297.2	494.1
PRODUCTION COSTS (\$/LB)					
RAW MATERIALS	34.94	30.45	32.05	34.94	41.86
BY-PRODUCTS	-1.83	-5.39	-2.87	-1.83	-0.08
UTILITIES	<u>9.51</u>	<u>9.51</u>	<u>11.21</u>	<u>7.77</u>	<u>17.56</u>
VARIABLE COSTS	42.62	34.57	40.39	40.88	59.34
LABOR COSTS	9.59	9.54	14.01	6.00	6.06
DIRECT COSTS	4.26	4.21	6.18	3.07	2.91
PLANT OVERHEAD, TAXES & INSURANCE	<u>11.48</u>	<u>11.38</u>	<u>16.66</u>	<u>7.64</u>	<u>8.17</u>
PLANT CASH COSTS	67.95	59.70	77.24	57.59	76.48
DEPRECIATION, 10%/YR OF TFC	<u>19.03</u>	<u>18.76</u>	<u>27.27</u>	<u>14.19</u>	<u>16.60</u>
PLANT GATE COSTS	86.98	78.46	104.51	71.78	93.08
G&A, SALES, RESEARCH	<u>15.00</u>	<u>15.00</u>	<u>15.00</u>	<u>15.00</u>	<u>15.00</u>
NET PRODUCTION COST	101.98	93.46	119.51	86.78	108.08
ROI BEFORE TAXES, 25%/YR OF TFC	<u>47.57</u>	<u>46.91</u>	<u>68.18</u>	<u>35.48</u>	<u>41.51</u>
PRODUCT VALUE	149.55	140.37	187.69	122.26	149.59

ECONOMICS FOR STAND-ALONE NYLON 6 PLANT WITH CAPTIVE PRECURSORS

	N66-SBU1	N66-SBU2	N66-SBU3	N66-SBU4	N66-SBU5 Case B
INVESTMENT (\$ MILLIONS)					
BATTERY LIMITS (BLI)	55.6	55.6	40.7	61.2	356.5
OFFSITES	<u>28.6</u>	<u>28.6</u>	<u>20.3</u>	<u>31.5</u>	<u>365.8</u>
TOTAL FIXED CAPITAL (TFC)	84.2	84.2	61.0	92.7	722.3
PRODUCTION COSTS (\$/LB)					
RAW MATERIALS	62.86	60.34	79.56	58.73	62.22
BY-PRODUCTS	--	--	--	--	-90.15
UTILITIES	<u>1.88</u>	<u>1.88</u>	<u>1.89</u>	<u>1.88</u>	<u>29.20</u>
VARIABLE COSTS	64.74	62.22	81.45	60.61	1.27
LABOR & OTHER FIXED COSTS	<u>5.49</u>	<u>5.49</u>	<u>8.03</u>	<u>4.94</u>	<u>21.38</u>
PLANT CASH COSTS	70.23	67.71	89.48	65.55	22.65
PLANT GATE COSTS	75.00	72.48	95.63	69.98	46.92
NET PRODUCTION COSTS	90.00	87.48	110.63	81.98	61.92
PRODUCT VALUE	101.93	99.41	126.00	93.05	122.60

Appendix A

PATENT SUMMARY TABLES

Table 4.1
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Preparation of Cyclohexanone									
CA 2285828	Bayer	10/16/98	Phenol	Supported Pd catalyst	140	0.5	3.0	100	94.5
Phenol is hydrogenated to cyclohexanone in the presence of Pt catalyst supported on activated carbon and sodium formate as a promoter.									
US 5395976	Bayer	12/18/92	Phenol	Supported Pd catalyst	150	0.5	?	100	>99.0 to KA oil
Phenol is hydrogenated to a mixture of cyclohexanone and cyclohexanol (KA oil) in the gas phase over Pd catalyst supported on Li-Al spinel and sodium formate as a promoter. The molar ratio of cyclohexanone to cyclohexanol (K/A molar ratio) in the reaction products can be controlled by specific treatment of the Pd catalyst during activation and regeneration. For the production of K/A ratio ranging from 85:15 to 98:2, the Pd catalyst has only initial hydrogen activation treatment, but with oxygen treatment followed by hydrogen treatment during regeneration of the catalyst activity. For the production of K/A ratio ranging from 30:70 to 85:15, the Pd catalyst requires both oxygen and hydrogen treatments during initial activation and later regeneration.									
US xxxx	Mitsubishi Chemical	7/19/96	Hexene	SiO ₂ /Ga ₂ O ₃ Cu ₂ O ₃ /Cr ₂ O ₃	120 250	0.1 0.17	1 2.4 hr ⁻¹	-- --	10.8 (yield) 60.0 (yield)
Cyclohexene is hydrated to cyclohexanol in an autoclave at 120°C under nitrogen in the presence of gallium silicate (atomic ratio of SiO ₂ /Ga ₂ O ₃ = 50:1). Cyclohexanol is dehydrogenated to cyclohexanone in a tubular reactor packed with a copper oxide-chromium oxide catalyst at 250 °C and 0.17 MPa. Cyclohexanone is purified in a series of three distillation columns.									
Preparation of Cyclohexanone Oxime									
US 5599987	Arco	3/31/95	Cyclohexanone	Titanium silicate	--	--	--	--	--
US 5451701	Chemical Technology	6/27/94							
An integrated process for producing cyclohexanone oxime is cited. The main reaction is ammoniation of cyclohexanone with ammonia and aqueous hydrogen peroxide solution in the presence of titanium silicate (titanium silicalite or titanosilicate) with molar ratio of Si:Ti ranging from 9.5:1 to 99:1. The molar ratio of hydrogen peroxide to cyclohexanone is preferably from 0.8:1 to 1.5:1. Excess ammonia is used relative to cyclohexanone at least 1.5:1 by mol. Methanol, t-butanol, or mixture thereof is used to form a single liquid-phase reaction mixture. The hydrogen peroxide solution is prepared by oxidation of isopropanol with air at 100-180°C with or without catalyst. The unreacted isopropanol and acetone by-products are removed by fractionation before the hydrogen peroxide is used for the ammoniation. The recovered acetone is subjected to hydrogenation to regenerate isopropanol.									
US 5684201	BASF	6/223/94	Cyclohexanone cyclohexanoneimine	TiO ₂ or γ -alumina Ti(BuO) ₄	80 100	10.0 5.0	-- 20	100 100	92-95 46
Cyclohexanone reacts with excess ammonia in a fixed bed reactor packed with either TiO ₂ or γ -alumina to form cyclohexylideneamine (cyclohexanoneimine) and water. The reaction mixture is mixed with chlorobenzene, and the resulting mixture is distilled to remove excess ammonia, and the resulting mixture is decanted to separate the aqueous layer. The cyclohexylideneamine in chlorobenzene is subjected to oxidation with air in the presence of Ti(BuO) ₄ (1 g catalyst per 10 g cyclohexylideneamine) to produce cyclohexanoneoxime.									

Table 4.1 (Continued)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Preparation of Cyclohexanone Oxime (concluded)									
US 5312987	Enichem Anic	4/1/92	Cyclohexanone	Ti-silicalite	85	0.23	1.2	98.3	99.6
A two-step process for producing cyclohexanone oxime is claimed. Initially, cyclohexanone in t-butanol reacts with hydrogen peroxide and ammonia in the presence of the titanium catalyst in microspheroidal form, which is suspended in the liquid media. The reaction product from the first step contains residual cyclohexanone, which further reacts with an aqueous solution of hydroxylamine in the second step for about 30 min to achieve nearly complete conversion of the residual cyclohexanone.									
US 5227525	Enichem Anic	1/23/91	Cyclohexanone	Ti-silicalite Ti-silicalite 85	85 85 85	0.28 0.23 0.18	1.0 1.0 0.5	97.8 ~98.0 ~100.0	>99.0 >99.0 >99.0
A three-step process for producing cyclohexanone oxime is claimed. Initially, cyclohexanone in t-butanol reacts with hydrogen peroxide and ammonia in the presence of the titanium catalyst in microspheroidal form, which is suspended in the liquid media. The reaction product from the first step is then fed to a second reactor along with additional cyclohexanone, hydrogen peroxide solution and ammonia. The reactor effluent from the second reactor is fed to a third reactor, where it further reactor with additional hydrogen peroxide to convert the residual cyclohexanone to cyclohexanone oxime.									
US 5900482	Mitsubishi Chemical	7/19/96	Cyclohexanone	Hydroxylamine sulfate	85	--	--	--	--
Cyclohexanone is converted to cyclohexanone oxime with aqueous ammonia in an autoclave in the presence of hydroxylamine sulfate. Cyclohexanol is dehydrogenated to cyclohexanone in a tubular reactor packed with a copper oxide-chromium oxide catalyst at 250 °C and 0.17 MPa.									
Beckmann Rearrangement of Cyclohexanone Oxime									
US 5264571	BASF	9/30/92	Cyclohexanone oxime	Oleum	85-125	--	--	~100	92-97
Rearrangement of cyclohexanone oxime is carried out in three stages with 60-85 wt% of cyclohexanone oxime and all oleum being added to the first stage. The remaining amount is added in decreasing ratio to the following stages. The oleum has 27-32 wt% SO ₃ . The holding time in each stage is about 10-60 min. About 20 vol% of the stream from the third stage is recycled to the second stage. The CAPM thus produced is neutralized with ammonia, and decanted to separate the ammonium sulfate solution. The crude CAPM is purified by extraction and distillation. The resulting CAPM has a permanganate titration number (PTN) of 16 as compared with 19 without recycling the stream from the third stage. PTN is determined by dissolving 1 kg CAPM in 2500 ml of 50 wt% sulfuric acid at 20°C. The solution is treated with 0.1 N potassium permanganate until a stable pink color is produced. The PTN is equivalent to the number of ml of potassium permanganate solution used. The lower the PTN is, the better the CAPM quality.									
US 6051706	Degussa-Huls	5/14/98	Cyclohexanone oxime	Zeolite catalyst	300	0.01-0.1	WHSV= 0.33 hr ⁻¹	--	92-97
Cyclohexanone oxime is dissolved in ethanol, and then evaporated and fed into a fixed-bed reactor packed with the zeolite catalyst supported on aluminosilicate. The catalyst is pentasil zeolite									
US 6071844 US 5741904	Degussa-Huls	5/4/95	Cyclohexanone oxime	Zeolite catalyst	300	0.01	WHSV= 0.25 hr ⁻¹	97->99	88-92
Cyclohexanone oxime is dissolved in ethanol (ethanol/oxime 9:1 by weight) and any additive components, and then evaporated and fed along with a carrier gas into a fixed-bed reactor packed with the boron-containing pentasil zeolite catalyst.									

Table 4.1 (Continued)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	Conversion %	Selectivity %
Beckmann Rearrangement of Cyclohexanone Oxime (concluded)									
US 5571913	DSM	8/20/93	Cyclohexanone oxime	--	--	--	--	--	--
Cyclohexanone oxime undergoes Beckmann rearrangement in the presence of lactam-o-sulfonic acid and cation exchange resin									
US 5900482	Mitsubishi Chemical	7/19/96	Cyclohexanone oxime	25% fuming sulfuric acid	90-125	0.1	2	--	--
Cyclohexanone oxime is subjected to Beckmann rearrangement with fuming sulfuric acid.									
US 6258949 B1 US 6265574 B1	Sumitomo Chemical	3/16/99 2/9/99	Cyclohexanone oxime	A zeolite catalyst	350	0.1	2	99.6	95.7
Cyclohexanone oxime is subjected to gas-phase Beckmann rearrangement in a fluid-bed reactor packed with zeolite granular of 0.3 mm in diameter. A second fluid-bed catalyst regenerator is connected to the main reactor. The reaction effluent from the fluid-bed reactor passes to a fixed-bed after-reactor, where residual cyclohexanone oxime is further converted to CAPM. The reaction effluent from the fixed-bed reactor contains 1000 ppm oxime based on CAPM as compared with 4000 ppm without the after-reactor. A spare fixed-bed after-reactor is installed in parallel for regeneration of deactivated catalyst.									
CAPM from Butadiene via 6AMCN									
Hydrogenation of Adiponitrile									
US 6222059	BASF	9/1/97	Adiponitile (ADN)	Fe/Fe oxide catalyst from magnetite and promoters	80-97	25	1.2-3.3	47-92	99 (to 6AMCN + HMDA)
ADN is partial hydrogenated in a series of three fixed-bed packed with the Fe/Fe oxide catalyst. Promoters include 1.3-1.9 wt% based on the catalyst of nitrate of Al, Si, Ti or V, and 1.03-1.04 wt% of hydroxide of Na, K, Li or Mg. The selectivity to 6AMCN decreases from 80% to 46% as the reaction temperature increases from 80 to 97°C.									
US 6207851	BASF	8/21/97	Adiponitile (ADN)	CoO catalyst	70	20	--	67	99 (to 6AMCN + HMDA)
ADN is partial hydrogenated in a tubular reactor packed with the catalyst comprising 90 wt% CoO, 5 wt% Mn ₂ O ₃ , 3 wt% P ₂ O ₅ and 2 wt% Na ₂ O. The catalyst is activated with hydrogen up to 280°C before the reaction. The resulting reaction mixture, consisting essentially of 32 wt% ADN, 48 wt% 6AMCN and 19 wt% HMDA, is distilled in a series of columns to separately recover HMDA and 6AMCN.									
US 6147247 US 6147208	BASF	8/21/97 12/22/95	Adiponitile (ADN)	Supported Co or Ni catalyst	120	4-8	1.2-3.3	70	99 (to 6AMCN + HMDA)
Butadiene is hydrocyanated in the presence of a complex of nickel with a triphenyl phosphine or phosphite ligand. The reaction mixture is treated either by extraction with alkali metal hydroxide or adsorption (or chemisorption) with calcium oxide to reduce the phosphorus content to less than 1 ppm based on ADN. The treated mixture is subjected to hydrogenation in the presence of ammonia and lithium hydroxide in a fixed-bed reactor packed with Co or Ni catalyst supported on alumina-silica, containing Mn ₂ O ₃ , Ag ₂ O, MgO, and/or CaO as promoters. The resulting hydrogenation product is distilled in a series of five columns to recover 6-aminocapronitrile (6AMCN) and hexamethylenediamine (HMDA).									

Table 4.1 (Continued)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	Conversion %	Selectivity %
Hydrogenation of Adiponitrile (continued)									
US 6080883 US 5874607	BASF	4/4/97 4/11/96	Adiponitrile (ADN)	Ni-containing catalyst	50-80	7.0-20.0	?	45-55	80-90 (selectivity to 6AMCN)
ADN is hydrogenated to produce 6AMCN and HMDA. The hydrogenation can be carried out in an upflow or downflow fixed bed reactor or in a suspension autoclave. The catalyst can be Raney nickel or Ni catalyst supported on silica. In the suspension process, the reaction takes place at 80°C and 7 MPa. Ammonia serves as a solvent at 1-6 g per g of ADN with a catalyst space velocity of 0.3-1.0 kg ADN per liter per hr. The catalyst is deactivated after 225 min. with the conversion of ADN reduced to 5%. The catalyst is reactivated by rinsing with liquid ammonia followed by treatment with hydrogen at 250°C for 5 hr. In the fixed-bed process, the reaction takes place at 50°C and 20 MPa. The conversion of AND dropped from 45% to 20% over a period of 280 hours while the selectivity to 6AMCN rose from 80 to 90%.									
US 6169199	BASF	2/7/97	--	--	--	--	--	--	--
A reaction product from hydrogenation of ADN contains 48 wt% 6AMCN, 0.27 wt% HMDA, 0.061 wt% tetrahydroazepine (C6H11N), and remainder of ADN. The mixture is distilled to recover HMDA in a column, of which top 1/3 trays are bubble cap, and the remainders are woven packing trays.									
US 6110856	BASF	9/10/96	ADN	Co/Fe catalyst	80	20.0	<1.0	75	50 (to 6AMCN) 50 (to HMDA)
A catalyst precursor consisting of 48 wt% CoO, 0.6 wt% of NaO, and 51.4 wt% F2O3 is packed in a tubular reactor. It is activated at 230°C and atmospheric pressure with a mixture of H2 and N2 for > 8hr, and 250°C and atmospheric pressure with pure H2 for additional 12 hr. The heat of reaction is removed through an external cooler in a circulation line. The selectivity is 50% to 6AMCN and 50% to HMDA.									
US 5789621	BASF	8/8/96	ADN	Co Fe	45-85 110-135	20 25	~0.75 ~0.75	70 70	>99.0 >99.0 (to 6AMCN and HMDA)
ADN is hydrogenated to produce 6AMCN and HMDA. The hydrogenation can be carried out in an upflow or downflow fixed bed reactor. The preferred catalyst is an unsupported Co and/or Fe catalyst containing a Co and/or Fe content of at least 60 wt% based on the total mass. The Co catalyst is activated with nitrogen at 280°C for 48 hr, while the Fe catalyst is activated at 370°C and 15 MPa first with nitrogen and then with hydrogen. After operation of 8000 hr, the Co catalyst deactivated, resulting in reduction of selectivity to 6AMCN from 50% to 23%. Similarly, the Fe catalyst is deactivated after 800 hr of operation. The deactivated catalyst is regenerated with hydrogen at 350-380°C and 20 MPa for 24 hr.									
US 5717090	BASF	1/5/95	ADN	Raney Ni and LiOH or Co catalyst	80 42-80	7.0 20	1.0 ?	54 60	95 (to 6AMCN) 5 (to HMDA) 60 (to 6AMCN) 40 (to HMDA)
ADN is hydrogenated to produce 6AMCN and HMDA. in a stirred tank reactor in the presence of a suspended Raney nickel and LiOH or in a tubular reactor packed with a Co catalyst promoted with Mn, P, Na metals. The resulting reaction mixture is subjected to a series of six distillation columns to separately recover 6AMCN and HMDA. The recovered 6AMCN is further cyclized to CAPM at 230°C 8.0 MPa for 15 min in a tubular reactor packed with TiO2 extrudates. The conversion of 6AMCN is complete with selectivity to CAPM of about 90%.									

Table 4.1 (Continued)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY									
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	Conversion %	Selectivity %
Hydrogenation of Adiponitrile (concluded)									
US 5508465	BASF	1/3/95	ADN	Ni Catalyst supported on alumina	160-200	0.09-0.5	--	23-95	91-59 (to 6AMCN)
The catalyst is prepared by adding aqueous Ni-nitrate solution to alumina extrudates at room temperature. After drying for 16 hr at 120°C and for 4 hr at 350°C, the catalyst is cooled and flushed for 2 hr with nitrogen. It is then activated with hydrogen at 300°C for 20 hr. The resulting catalyst contains about 13 wt% Ni, and can be doped with alkali metal at the amount of 0.1 wt%.									
US 6114567	BASF	12/27/94	ADN	Co catalyst or Ni catalyst	60	18-20	--	50-80	78
US 5801268									to 6AMCN
US 5801267									G100
US 5756808									to 6AMCN+ HMDA
ADN is hydrogenated in a fixed bed reactor packed with solid catalysts containing mainly cobalt, nickel or ruthenium along with promoters, such as Mn, P, Ag, Fe, Ca, Na, and Mg. The catalysts are prepared from the oxides of these metals, and are activated at 280°C for 48 hr under hydrogen.									
US 5844114	DSM	5/14/93	ADN	Ni-ZSM34 or Ni-SAPO34	120-140 110-125	7.0-8.0 7.0-8.0	1-5 2-19	65-67 11-75	40-100 to 6AMCN 60-0 to CAPM 62-100 to 6AMCN 38-0 to CAPM
Two nickel catalysts are used for partial hydrogenation of ADN to 6AMCN and CAPM. The Ni-ZSM34 is prepared from a gel having a composition, expressed in molar ratios: Si/Al = 9.5, Na/Al = 5.8, and K/Al = 1.2. The gel is heated to 190°C in an autoclave, and then precipitates after cooling. The solid is washed with water, and contacted with ammonium nitrate at 180°C and then with nickel nitrate at 80°C. The resulting solid is calcined in the air at 540°C for 3.5 hr to get Ni-ZSM34. The Ni-SAPO34 is prepared similarly with a gel having a composition of Si _{0.15} Al _{1.0} TEA _{1.03} Ni _{0.15} H ₂ O ₃₉ . When Ni-ZSM34 is used, the selectivity to HMDA decreases as the reaction time increases. The reverse is true when Ni-SAPO34 is used.									
US 5723603	Rhone-Poulenc Fiber & Resin Intermediates	6/17/96	ADN	Raney nickel containing 1.7 wt% Cr.	50	2.0	2-3.5	81-85	60-64
ADN is partially hydrogenated to 6AMCN in HMDA in the presence of the Ni catalyst and small amounts of alkali metal hydroxide. After separation of the catalyst by filtration, the filtrate is distilled to obtain 6AMCN with 97-98 wt% purity. The 6AMCN is then subjected to cyclizing hydrolysis in a vertical reactor packed with alumina. Quartz is added to the sections above and below the quartz packing. The reaction takes place at 320°C with a mixture of 6AMCN and water (water/6AMCN molar ratio of 1.1:1) injected into the reactor. The conversion of 6AMCN is reported at 63 % with selectivity of 100% to CAPM.									
US 5981790	Rhone-Poulenc Fiber & Resin Intermediates	12/14/94	ADN	Raney nickel	50	2.0	1.33	71-83	68-77
ADN is partial hydrogenated to 6AMCN in a mixture of HMDA and water in the presence of Raney nickel and a small amount of KOH.									

Table 4.1 (Continued)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY									
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	Conversion %	Selectivity %
Hydroformylation of Pentenenitrile									
US 6048997	BASF	8/31/96	Pentenenitrile	Co ₂ (CO) ₈ Rh(CO) ₂ (acac)	170 100	2.8 0.5	2.0 5.0	>99.9 98.6-99.9	--
3-PN or 4-PN is hydroformylated in the presence of cobalt carbonyl catalyst or rhodium carbonyl catalyst to form 5-formylvaleronitrile (5-FVN) and other by-products, such as valeronitrile, 3- and 4- formylvaleronitriles, and 6-hydroxycapronitrile. After separation from these by-products, 5-formylvaleronitrile reacts with ammonia and hydrogen in the presence of Ru catalyst supported on alumina at 80°C and 7.0 MPa to form 6AMCN and HMDA.									
US 6121481	BASF	8/3/96	5-FVN	Ru, Pd or Co supported on alumina	80-100	7-10	>20	100	56-73
6AMCN is prepared from 5-FVN by reacting with ammonia and hydrogen in the presence of a hydrogenation catalyst, selected from metals of Fe, Co, Ni, Ru, Rh, or Pd.									
CAPM by Cyclization of 6AMCN									
US 5693793	BASF	7/17/96	6AMCN	TiO ₂ extrudate	225	10.0	0.25	98	92
ε-Caprolactam (CAPM) is prepared by cyclization of 6AMCN in the presence of a mixture of water and ethanol through a fixed-bed reactor. The reactor effluent is distilled to remove ammonia, ethanol and water. The resulting crude CAPM is further distilled under reduced pressure to remove low boilers, essentially ethyl 6-aminocaproate and unconverted 6AMCN, and high boilers, essentially oligomers. The latter can be depolymerized to CAPM using phosphoric acid or polyphosphoric acid with or without steam.									
US 5874575	BASF	12/3/94	6AMCN	TiO ₂ extrudate	200	10.0	0.5	100	--
CAPM is prepared from 6AMCN in a mixture of water and ethanol (3.2-16 wt% water) and in the presence of titanium oxide in the form of 1.5 mm extrudates. The reaction takes place in a fixed-bed reactor. The reaction mixture is distilled or gas purged to remove ammonia along with some water. The resulting residue is further distilled to separate light ends and heavy ends from CAPM. The light ends are ethyl 6-aminocaproate, and unconverted 6AMCN while the heavy ends are 6-aminocaproamide, 6-aminocaproic acid, and oligomers of CAPM.									
US 5495014	BASF	12/1/94	6AMCN	TiO ₂ extrudate	200	10.0	0.5	100	88
6AMCN is converted to CAPM by cyclization of a mixture of 10 wt% 6AMCN, 6.4 wt% water, and 83.6 wt% ethanol in a tubular reactor packed with titanium dioxide (anatase). The reaction effluent is distilled to recover CAPM as a distillate with a bottom stream containing 9 wt% oligomers, 1 wt% CAPM, 6.4 wt% water, and remainder of ethanol. The bottom stream is subjected to decomposition at 230°C 10.0 MPa through a tubular reactor also packed with TiO ₂ extrudate.									
US 5495016	BASF	11/25/94	6AMCN	--	300	--	1.0	100	~76
6AMCN in an aqueous solution is heated at 300°C for 1 hr to be converted to a mixture of 76 wt% CAPM and 24 wt% oligomers without catalyst. The reaction mixture is vacuum distilled under 100-300 mbar to remove ammonia and water with the bottom stream being further distilled the a second column under 3-10 mbar. 97.3 % of the CAPM in the reactor mixture is recovered as a distillate from the second column.									

Table 4.1 (Continued)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	Conversion %	Selectivity %
CAPM by Cyclization of 6AMCN (concluded)									
US 5739324	BASF	11/20/93	6AMCN	TiO ₂ pellets	180-240	0.5-15	0.5	98-100	88-98
CAPM is prepared by reacting 6AMCN with water in the presence of a heterogeneous catalyst selected from TiO ₂ , ZrO ₂ CeO ₂ and Al ₂ O ₃ . The amount water to 6AMCN is preferably 1:1-5:1 by mol, or 5-30 wt% 6AMCN in aqueous solution or in a mixed solvent of water and ethanol (water:ethanol = 1:99 – 50:50).									
US 5493021	Rhone-Poulenc Chimie	12/23/93	6AMCN	LaPO ₄ or AlPO ₄	320	--	50-100 seconds	<90	<92
CAPM is prepared by reacting 6AMCN with water in vapor-phase in a fixed-bed reactor packed with LaPO ₄ in between two layers of quartz packing. The LaPO ₄ calcined at 700°C for 4 hr provides a conversion of 90% with 92% selectivity. But the activity of this catalyst deteriorates over a period of 25 hours. LaPO ₄ doped with cesium hydrogenphosphate longer linger live than the other catalysts.									
CAPM from Butadiene									
WO 00/37431	Rhodia Fiber and Resin Intermediates	12/22/98	Butadiene	Ni(COD)2 and a water soluble phosphine	90	1.5-9.0	1.5	95	91.5
Methyl-2-butene-3-nitrile is isomerized to 3-pentenenitrile (3-PN) in the presence of Ni(COD)2 and sodium triphenylphosphine trisulfonate.									
CAPM from Butadiene via 6AMCA, 6ACAM and M6AMC									
Carbonylation of Butadiene									
US 6175036	DSM	2/26/97	Butadiene	Acidic ion exchanger	120	4.0	6	--	--
			3-methyoxy-1-butene	Pd-acetate and promoters	140	5.0	1	47	>98
Methyl-3-pentenoate is prepared from butadiene via 3-methyoxy-1-butene. The promoters are bis(diphenylphosphino)butane, 2,4,6-trimethylbenzoic acid, and otho-dichlorobenzene.									
US 5495041	DSM and DuPont	2/22/95	Butadiene	Pd(II)-acetate, Ligand and acid	140	6.0	2	75	79
Methyl-3-pentenoate is prepared from butadiene by carbonylation of butadiene in the presence of methanol, and a catalyst system comprising Pd catalyst, a bidentate phosphine ligand, such as the one shown in US 6175036, and 3-pentenoic acid. The molar ratio of the carboxylic acid to Pd catalyst is 10:1. During the reaction, about 46-70% of the acid is converted to methyl ester. In the process, a part of the methyl-3-pentenoate is hydrolyzed to 3-pentenoic acid, which is recycled to the reactor to maintain a catalytically active level for the reaction.									
US 5693851	DSM and DuPont	8/23/93	Butadiene	Pd(II)-acetate, Ligand and acid	130-150	6.5	4.5-5.0	80-90	91-96
Methyl-3-pentenoate is prepared from butadiene and methanol by carbonylation in diphenyl ether. A bidentate phosphine ligand, such as 1,1'-bis(disopropylphosphino)furanocene, 1,1'-bis(disobutylphosphino)furanocene, or 1,1'-bis(cyclohexylphosphino)furanocene, is used to react with Pd-acetate to form catalyst precursor to improve the conversion of butadiene. 2,4,6-trimethylbenzoic acid or pentenoic acid can be used as the acid for the reaction. After the carbonylation, the reaction effluent is sent to a flasher, where CO is separated. The resulting liquid mixture is distilled first to recover unreacted butadiene and methanol, which are recycled to the reactor. The crude pentenoate is further distilled to recover purified pentenoate. The bottom stream, containing the catalysts high boiling by-products and solvent, is subjected to crystallization to recover the catalysts, which is recycled to the reactor.									

Table 4.1 (Continued)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	Conversion %	Selectivity %
Hydroformylation of Methyl Pentenoates									
US 6030505	BASF	8/9/95	--	--	--	--	--	--	--
The difference in the boiling points for M-5FV and M-4FV is only 2.4°C. This makes separation of M-5FV from its isomers by distillation at atmospheric pressure very difficult. In the present process, a mixture of formylvaleric acid esters from the hydroformylation of a mixture of 3-and/or 4-pentenoic acid esters is distilled in a series of three columns operated under reduced pressures to recover methyl 5-formylvalerate (M-5FV) with a yield ≥ 90%.									
US 5719312	DSM	12/30/93	3-Pentenoic acid or its ester	Rh(CO) ₂ (acac) catalyst and phosphite ligand	90	1.0	26-27	45-54	78-80
3-Pentenoic acid or its methyl ester is hydroformylated to form M5FV, which can be converted to CAPM as indicated in US 5973143. The ligand is bidentate phosphite.									
US 5527950	DSM and DuPont	1/6/94	Freshly distilled methyl-3-pentenoate (M3P) or a mixture of pentenoates	Rh(AcAc)(CO) ₂ and phosphine ligand	110	1.0	2 21	17.5 82	79 77
M5FV is prepared by hydroformylation of methyl pentenoates in the presence of Rh carbonyl catalyst and a phosphine ligand. The phosphine ligand is sodium salt of tris(m-sulfonatophenyl)phosphine. The presence of trace amount of oxygen in the reaction system will cause the formation of hydroperoxide compounds through the reaction of oxygen with methyl pentenoates, particularly methyl-2-pentenoate. Reportedly, the freshly distilled M3P contains <40 ppm, and the mixture of methyl pentenoates contains 12500 ppm. The presence of hydroperoxide compounds converts the phosphine ligands into catalytically inactive compounds. Therefore, it is necessary to pre-wash the mixed pentenoates with an aqueous solution of sodium tris(m-sulfonatophenyl)phosphine before the hydroformylation.									
US 5698745 US 5618983	DuPont	8/25/95	Methyl-4-pentenoate (M4P)	Pt(AcAc) and a ligand	100	6.9	80	85-89	89-92
Methyl-4-pentenoate is hydroformylated to methyl-5-formylvalerate in the presence of Pt(AcAc) and a ligand selected from 1,1'-bis(diphenylphosphino)ferrocene, 1,1'-bis(diphenylphosphino)ferrocene, and 1,1'-bis(diphenylphosphino)-3,3-bis(trimethylsilyl)ferrocene.									
Reductive Ammoniation of M5FV									
US 5877314	DSM and DuPont	2/14/97	M5FV	Ru on titanium oxide	120	4.0	~1.0	~100	97 CAPM and its precursors
M5FV is prepared by formylation of pentenoate esters as described in US 5527950. It is subjected to a combined hydrolysis and reductive ammoniation in a single reactor to produce CAPM and its precursors, such as 6AMCA, 6ACAM and M6AMC. The Ru catalyst is pre-reduced at 140°C for 12 hr. The titanium oxide carrier with a higher BET surface area, i.e. 48 m ² /g provides a 3.5 times higher catalyst activity than that with 3.4 m ² /g. The reaction is carried out continuously in a Hastelloy-C autoclave. The catalyst activities for Ru on alumina support or Raney nickel decrease rapidly after initial short period of reaction.									
US 5973143 US 5780623	DSM	2/23/96	M5FV	Ru on alumina or Raney nickel	100-120	1.5-3.0	--	~100	96-97 CAPM and its precursors
M5FV is subjected to a combined hydrolysis and reductive ammoniation at 100-120°C and 1.5-3.0 MPa in the presence of a catalyst selected from Ru on alumina and Raney nickel. The resulting mixture is steam stripped to remove ammonia and methanol. The stripped mixture, which comprises a mixture of CAPM, 6AMCA, 6-aminocaproamide (6ACAM) and oligomers, is subjected to cyclization at 300°C and 10 MPa. The reaction mixture is distilled in a series of two columns to recover CAPM.									

Table 4.1 (Continued)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	Conversion %	Selectivity %
Reductive Ammoniation of M5FV (concluded)									
US 5717089	DSM	3/1/95	M5FV	--	35	--	15 seconds	--	--
US 5700934	and DuPont			Ru on alumina or Raney nickel	120	< 3.0	1.0	~100	>99 CAPM and its precursors

M5FV is subjected to a combined ammoniation and reductive ammoniation in a series of two reactors. The reaction in the first reactor takes place without a hydrogenation catalyst, while the reaction in the second reactor takes place in the presence of a catalyst selected from Ru on alumina and Raney nickel. When Ru catalyst is used, the yield is 85-96.5% to methyl 6-aminocaproate (M6AC), and about 4% to CAPM. When Raney nickel is used as the catalyst, the yield is 59% to 6ACAM, 24-25% to 6AMCA, and 15-17% to CAPM. High selectivity to CAPM and its precursors can be achieved by keeping a molar ratio of water to ammonia at < 2:1, and hydrogen pressure at < 3 MPa.

US 5925754	Union Carbide	10/23/97	Butadiene	PdCl ₂ and (R) ₃ P	110	1.5-6.9	2	18-35	94-99
US 5962680		4/15/97		Rh(CO) ₂ (AA) and ligand	85	0.7	1-2	?	88-93
				Cr-promoted Raney Ni	220	4.8	3	?	?

CAPM is prepared from 1,3-butadiene in three steps of reactions. The butadiene is first converted to 3 & 4 pentenoic acid by hydroxycarbonylation in the presence of Pd catalyst and a trialkylphosphine ligand. Under 110°C and 1.5-6.9 MPa The pentenoic acid is converted to 5-formylvaleric acid by hydroformylation in the presence of Rh catalyst (dicarbonylacetone rhodium) and a phosphine ligand under 85-90°C and 0.7 MPa. The formylvaleric acid is finally converted to CAPM through reductive ammoniation in the presence of Cr promoted Raney Ni catalyst under 220°C and 4.8 MPa.

Cyclization of CAPM Precursors									
US 5502185	BASF	6/28/94	6-Aminocaproic acid (6AMCA)	TiO ₂ extrudate	220	10.0	0.25	97-100	95

CAPM is prepared by cyclization of 6AMCA in the presence of a mixture of water and ethanol through a fixed-bed reactor. The reactor effluent is distilled to remove ethanol and water. The resulting crude CAPM is further distilled under reduced pressure to remove low boilers, essentially ethyl 6-aminocaproate and unconverted 6AMCA, and high boilers, essentially oligomers.

US 6194572	DSM	2/19/97	An aqueous mixture of 6AMCA, its ester and/or 6ACAM	--	300	1.2	?	--	>99 (yield)
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The aqueous mixture of 6AMCA, its methyl or ethyl ester, and/or 6ACAM can be obtained from M5FV by a combined hydrolysis and reductive ammoniation as indicated in US 5973143, or from 6AMCN by hydrolysis. The mixture, which may also contain some CAPM and oligomers, is subjected to cyclization by contacting with a superheated steam. Part of the steam can be substituted with an inert stripping gas, such as nitrogen. The weight ratio of the steam to the aqueous mixture is preferably between 1:1 and 20:1. The reaction product is withdrawn as a vapor containing CAPM, steam and some ammonia when 6ACAM is present in the aqueous mixture. The vaporous product is partially condensed at 100-170°C to recover CAPM with some water, and the uncondensed steam can be reused in the process before ammonia if any is removed. The crude CAPM is purified by the method described in US 5496941.

Purification of Caprolactam									
US 5952493	BASF	12/18/97	--	--	--	--	--	--	--

Crude CAPM from either cyclization of 6AMCN or Beckmann rearrangement of cyclohexanone oxime is purified by reducing the impurities with sodium borohydride in the presence of water at <100°C for 24-100 hr before water and the reduced impurities are distilled off under a slightly reduced pressure. The resulting CAPM has a UV number of 3.1-3.5.

Table 4.1 (Continued)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	Conversion %	Selectivity %
Purification of Caprolactam (concluded)									
US 6011153	DSM and DuPont	2/23/96	An aqueous mixture from reductive ammoniation of 5FVA or M5FV	--	300	10	0.5-1.0	--	--
An aqueous mixture from reductive ammoniation of 5-formylvaleric acid (5FVA) or its methyl ester, M5FV, comprises 77.9 wt% water and 22.1 wt% organic compounds, which contains 14.2 mol% 6AMCA, 39.9 mol% 6ACAM, 33.9 mol% CAPM, and a remainder of oligomers. The oligomers are a mixture of linear dimers or trimers of 6AMCA, 6ACAM, and cyclic dimers and trimers of the same. The aqueous mixture is subjected to cyclization reaction at 300°C and 10 MPa for 0.5-1.0 hour. The resulting reaction effluent is distilled under a reduced pressure in a series of two columns to recover CAPM, which is a distillate from the second column. The residue from the bottom of the second column, containing unconverted CAPM precursors and some CAPM, is recycled to the cyclization reactor. The yield of CAPM is reported 77 mol%. In the present case, the CAPM yield is defined as the amount of CAPM in mol in the reactor effluent divided by the total mols of the aqueous mixture fed to the cyclization reactor.									
US 5496941	BASF	1/3/95	--	--	--	--	--	--	--
Crude CAPM prepared from cyclization of 6AMCN is first distilled to remove both high boilers and low boilers. The CAPM thus obtained has a purity of 99.5%, which is subjected to hydrogenation treatment at 80°C in the presence of water and a Pd catalyst supported on active carbon. The reaction mixture is filtered to remove the Pd catalyst. The filtrate passes over a highly acidic ion exchanger bed at 50°C. It is finally distilled through a series of three columns to first remove water and then low boilers and high boilers to obtain purified CAPM.									
US 5441607	BASF	7/9/93	--	--	--	--	--	--	--
A distillation residue from CAPM purification is heated to 315°C and thus melted. A steam at 350°C is then passed through the melt, which contains 46.3 wt% CAPM, 5 wt% sodium hydroxide, and remaining with oligomers, impurities and decomposition products. A vapor stream escaped from the vessel contains a mixture of water and CAPM, which is condensed to recover CAPM.									
US 5637700	BASF	9/8/92	--	--	--	--	--	--	--
Crude CAPM, containing CAPM and unsaturated lactams, such as 3,4- and 4,5-dehydrocaprolactam, by oxidative treatment at 80°C with oxygen or oxygen-containing gas mixture in an alkaline medium.									
US 6191274	DSM	2/17/96	--	--	--	--	--	--	--
Crude CAPM from cyclization of an aqueous mixture, which is derived from hydrolysis of 6AMCN, is extracted with chloroform or 4-methyl-2-pentanol to recover CAPM with no detectable 6ACAM, 6AMCA and oligomers found in the chloroform phase.									
US 5539106	DSM	7/19/93	--	--	--	--	--	--	--
Crude CPAM from Beckmann rearrangement is neutralized with ammonia and extracted with benzene four times. The resulting benzene extracts are combined and extracted with water two-three times. The resulting water phases from these extractions are mixed, and the resulting aqueous solution, containing 35 wt% CAPM is saturated with hydrogen before passing through a vertical tubular reactor packed with nickel catalyst supported on alumina/silica.									

Table 4.1 (Concluded)
TECHNOLOGY FOR CAPROLACTAM

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	Conversion %	Selectivity %
Purification of Caprolactam (concluded)									
US 6100396	Rhodia Fiber and Resin Intermediates	8/2/96	--	--	--	--	--	--	--
Crude CAPM from vapor-phase cyclization of 6AMCN is first distilled (or evaporated) at 90°C for 0.5 hr to remove ammonia along with a certain amount of water such that the resulting bottom stream has a solution with CAPM concentration not greater than 80 wt%. The CAPM solution, having CAPM concentration of less than 60 wt% is then extracted with a mixture of 30 wt% bis(2-ethylhexyl)hydrogen phosphate and 70 wt% cyclohexane. Alternatively, the solution is treated with an amount of macroporous sulphonic resin with a solution to resin ratio of 0.3:1 in equivalent to remove most of by-products. The crude CAPM thus treated is distilled to get purified CAPM for the production of nylon 6.									
US 6252068	Sumitomo Chemical	12/28/98	CAPM	Pd on active carbon	80-95	0.5	--	--	--
A mixture of cyclohexanone oxime, methanol and water (1:1.8:0.052 by weight) is subjected to gas-phase Beckmann rearrangement in a fluidized bed reactor at 380°C. Crude CAPM from Beckmann rearrangement is distilled to remove methanol, light ends and heavy ends. The resulting CAPM has a purity of 98.97 wt% with impurities of 584 ppm cyclohexanone oxime, 604 ppm of 3-N-methyl-4,5,6,7-tetrahydrobenzimidazole, and 355 ppm of 1,2,3,4,6,7,8,9-octahydrophenazine. It is dissolved in a mixed solvent of cyclohexane and n-heptane at 70°C followed by cooling to 50°C for 2 hr to precipitate CAPM with a yield of 94.8%. The crystallized CAPM is then melted and is in contact with hydrogen at 80-95°C and 0.5 MPa in a tubular reactor packed with a hydrogenation catalyst (granular 2 wt% Pd supported on active carbon) to get CAPM with >99.99% purity.									
US 5502184	Sumitomo Chemical	8/20/93	CAPM	Pd on active carbon	130-170	0.2-1.0	--	--	--
Crude CAPM from gas-phase Beckmann rearrangement is purified by rectification, extraction or crystallization. It is further treated hydrogen to achieve its purity to > 99.9%. The treatment can be carried out batchwise in an autoclave with a suspended catalyst, or continuously in a stainless steel column packed with catalyst pellets.									

Table 4.2
NYLON 6 BY HYDROLYTIC POLYMERIZATION

PATENT SUMMARY								
Reference Number (Patent)	Assignee	Earliest Date Shown	Water Concentration (pph)	Catalyst	Concentration (pph)	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)
WO 9926998	BASF	11/25/97	--	--	--	--	--	--
Nylon 6 granules from the polymerization are continuously extracted in a vertical extraction column having two operation zones to remove CAPM and oligomers. An aqueous 20-30 wt% CAPM solution is used as an extraction agent for the top zone under 115-130°C, and water is fed to the lower end of the bottom zone at 20-30°C.								
WO 9926996	BASF	11/25/97	--	--	--	--	--	--
Nylon 6 granules (from 1.5x1.5 mm to 4x4 mm) from the polymerization are continuously extracted in a vertical extraction column having two operation zones to remove CAPM and oligomers. An aqueous 75-95 wt% CAPM solution is used as an extraction agent for the top zone under 115-130°C, and water is fed to the lower end of the bottom zone at 20°C. The residence time for the polymer stream is 4-6 hr in the top zone, and 5-30 min in the bottom zone. The bottom zone is a slender and unheated tube.								
US 4879120	BASF	8/25/88	--	--	--	--	--	--
Nylon 6 having a relative viscosity of 2.7 and containing 11 wt% extractables (9 wt% CAPM and 2 wt% oligomers) and 0.27 wt% titanium dioxide is continuously extracted with demineralized water in countercurrent at a temperature range of from 115° to 125°C. Extracted nylon 6 contains 0.3 wt% titanium dioxide, 0.5 wt% extractables (0.1 wt% CAPM and 0.4 wt% cyclic oligomers), and 0.03 wt% water. The extract water containing 10.5 wt% CAPM and about 1.9 wt% oligomers is concentrated together with CAPM (8.8 wt% based on the extract water) by evaporation at 115-185°C and 0.11 MPa to a solid content of 98 wt%. The concentrate is recycled without purification to polymerization reactor along with fresh CAPM.								
US 4816557 EP 167975 A2	BASF	3/31/87 7/10/84	--	--	--	--	--	--
Nylon 6 granules from the polymerization are continuously extracted in a vertical extraction column, where the granules are treated with superheated steam of 170°C fed at the bottom of the column. The granules are preheated to 120°C with superheated steam before it is fed into the extraction column. From the top of the column a mixture of steam, CAPM and oligomers is removed and passes to a column to give a 60-70 wt% aqueous solution of CAPM and oligomers at the bottom, and virtually CAPM-free stream from the top. The aqueous solution is further concentrated to 90 wt% before it is recycled to polymerization operation.								
US 5703204	Bayer	5/31/95	--	--	--	--	--	--
The aqueous extract from Nylon 6 production is concentrated by evaporation. The resulting concentrated extract is recycled to polymerization along with 6-AMCA and small amount of adipic acid (ADA) at 1-6 mmol per kg of extract on dry basis. The addition of ADA provides the resulting polyamide with higher MW than polymerization of the extract without any addition of ADA.								
DE 4324616	Bayer	7/22/93	--	--	--	--	--	--
Nylon 6 granules from the polymerization are continuously extracted in a vertical extraction column with 42-60 wt% aqueous solution of CAPM at 80-120°C.								
US 5026818	Bayer	9/17/88	--	Tris-(2,4-di-t-butyl)phenyl phosphite	0.56	200 270	? 1.0 1.3	
The melt condensation polymerization for the production of high MW nylon 6 is carried out in the presence of a mixture of additives including α -amino- ϵ -caprolactam (ACL) and/or lysine (or lysine hydrate), to increase the polymerization rate.								

Table 4.2 (Continued)
NYLON 6 BY HYDROLYTIC POLYMERIZATION

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Water Concentration (pph)	Catalyst	Concentration (pph)	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)	
US 6069228	DuPont	8/17/98	25	--	--	--	--	--	
				An aqueous CAPM solution of 80 wt% is fed continuously into a vertical coiled pipeline reactor. The reactor coils are submersed in an oil bath operated at 272°C. The prepolymerization takes place under 2.8 MPa, which is below the solution vapor pressure to allow formation of a steam phase. The residence time for the liquid prepolymer is 35-40 min. The resulting two-phase reactor effluent enters a flasher at 270°C with a residence time of 2-3 min before it passes to a separator, where a steam-monomer mixture is separated from the prepolymer. The residence time for the liquid phase in the separator is less than 1 min. The molten prepolymer is then crystallized either through a steel belt, which is heated at a controlled temperature below the melting point of the prepolymer, or quenched with water at a temperature near or above the nylon 6 glass transition temperature of 60°C. It is reported that an increased α -crystalline morphology occurs in the solid prepolymer when the molten prepolymer is quenched at a temperature well above the glass transition temperature. An increased γ -crystalline morphology occurs in the solid prepolymer when the molten prepolymer is quenched at a temperature near the glass transition temperature. The prepolymer with α -crystalline morphology is more suitable for solid-phase polymerization. The crystallized prepolymer is subjected to solid-phase polymerization in a vertical tubular reactor with a conical bottom section. The polymer flow downward countercurrently with heated nitrogen gas at 160°C.					
US 6093788	Lurgi Zimmer	12/2/97	--	--	--	--	--	--	
				\square CAPM is recovered from the extract water from a hydrolytic polymerization for nylon 6. The extract water is first concentrated from 8 wt% to 70 wt% by means of multi-stage distillation. The concentrated extract water is further distilled or evaporated to recover a CAPM/water mixture, and to yield an extract containing 33-67 wt% CAPM and 67-33 wt% oligomers (including dimers). The latter is depolymerized in the presence of a catalyst and superheated steam to generate a vaporous mixture of 16-33 wt% CAPM and 84-67 wt% water, which is condensed and combined with the CAPM/water mixture from earlier evaporation.. The resulting CAPM/water mixture is distilled to yield CAPM with a water content of less than 4 wt% and a dimer content of not greater than 0.05 wt%.					
US 5777067	Mitsubishi Chemical Kasei	11/6/95	2.5	--	--	250 250	0.7 450 (mmHg)	2.0	
				Fresh CAPM is combined with recycled mixture of unreacted CAPM and oligomers. The resulting mixture is subjected to hydrolytic polymerization to form nylon 6, which is pelletized and extracted with hot water. The resulting aqueous solution from the extraction is condensed to 75-95 wt%, and recycled to the polymerization along with the fresh CAPM.					
JK 05331281	Mitsubishi Chemical Kasei	5/29/92	--	--	--	270 270	0.5 450 (mmHg)	?	
				An extract water from nylon 6 chips, which contains 8 wt% unreacted CAPM, 1 wt% oligomers, and fine silica particulate, is treated with a strong cationic ion exchange resin followed by anionic ion exchange resin at 40°C. The extract water is then concentrated to 90 wt% followed by distillation to recover CAPM with 80 % yield.					
US 5973105 US 5962538	Polymer Engineering	8/30/95 8/30/95	--	--	--	--	--	--	
				An extract water from nylon 6 production is concentrated to an average solid content of 93 wt%. This is heated to 150°C to assure that all dimers and oligomers are dissolved. The resulting solution is further heated to 240°C, and then fed to a dimer treatment stage along with some water (to a water content of 6 wt%). The cyclic oligomers, especially dimers are cleaved by hydrolysis. The cleaved mixture is polymerized along with fresh CAPM at equal amount to produce nylon 6.					
JK 11343338	Toray Ind.	6/2/98	100	Phosphoric acid	0.033	380	25	3	
				CAPM is hydrolyzed in a critical state in the presence of phosphoric acid with 94% of CAPM converted to α , ω -aminocaproic acid. The amount of water is reduced to 46.6 pph when the reaction is carried out under 1400 pph CO ₂ at 250°C and 15 MPa. In this case, 93% of CAPM is converted. The resulting α , ω -aminocaproic acid is recovered, and it is mixed with CAPM at 0.433 pph based on CAPM. The resulting mixture is polymerized at 230°C for 5 hr to produce nylon 6.					

Table 4.2 (Concluded)
NYLON 6 BY HYDROLYTIC POLYMERIZATION

PATENT SUMMARY								
Reference Number (Patent)	Assignee	Earliest Date Shown	Water Concentration (pph)	Catalyst	Concentration (pph)	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)
US 6169161	Toray Ind.	4/3/98	100	Phosphoric acid	0.033	223-245	--	--
CAPM is polymerized in two steps. In the first step, CAPM is polymerized under atmospheric pressure into a product of which the content of unreacted CAPM is not higher than 10 wt% and that of oligomer is less than 2 wt%. To remove the unreacted CAPM and oligomer the reaction effluent is sent to a vented twin-screw extruder at a temperature ranging from 160°C starting from the feeder to 260°C in the second step. Alternatively, it can be sent to a thin film evaporator equipped with multi-stage stirring blades at 250°C and 1 mmHg, or a double-coned vacuum drier under reduced pressure in a solid-phase state.								
JK 02024322	Toyobo KK	7/12/88	--	--	--	--	--	--
An extraction column having an L/D ratio of 30-35:1 is used for extracting CAPM and oligomers from nylon 6 chips. The extraction is conducted at 110-120°C and 0.2-0.4 MPa for about 5 hr.								
JK 01259035	Ube Ind.	4/11/88	5	--	--	260	?	9
Modified nylon 6 having hydroxyphenyl end groups are prepared by adding small amount of p-hydroxyphenyl stearate to the reaction mixture. The resulting polyamide considerably less water-absorption than the polyamide without the additive.								

Table 4.3
NYLON 6 BY ANIONIC POLYMERIZATION

PATENT SUMMARY

Table 4.4
TECHNOLOGY FOR ADIPIC ACID

PATENT SUMMARY										
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)	
Adipic acid from Benzene										
Partial Hydrogenation of Benzene										
US 5973218	Asahi Kasei	7/8/97	Benzene	Ru catalyst promoted with aq. zinc sulfate	130	5.0	--	30-70	82-84.5	
Cyclohexene is prepared from benzene in slurry by partial hydrogenation in the presence of Ru catalyst with zinc sulfate serving as a promoter. To maintain the activity of the catalyst during the reaction, the concentration of the zinc salt is kept initially at 0.5 mol/l, and increased to 0.8 mol/l after 1600 hours of operation.										
US 5589600	BASF	2/5/92	Benzene	Ru catalyst modified with nickel	150	5.0	15-30 min	20-44	66-76	
Cyclohexene is prepared from benzene by partial hydrogenation in water in an autoclave in the presence of suspended nickel modified Ru catalyst with promoters, such as aqueous ZnSO ₄ and ZnO ₂ . The volume ratio of water to benzene used in the reaction is 95:45. The amounts of ZnSO ₄ and ZnO ₂ is 32 and 4 g per g of the catalyst.										
US 5639927	Mitsubishi Chemical	12/19/94	Benzene	Ru catalyst supported on silica modified with	150	5.0	30-42 min	30-63	70-81	
US 5569803		12/24/93		ZrO ₂						
Cyclohexene is prepared from benzene by partial hydrogenation in water in the presence of Ru catalyst supported on zirconium oxide-modified silica. The solid catalyst contains about 0.05-5 wt% Ru. The catalyst is pretreated with ZnSO ₄ or LiSO ₄ at 150-200°C for 5 hours followed by hydrogen treatment. The treated catalyst is washed with water and dried. The dried catalyst is further treated with hydrogen at 200°C for 2 hours before it is used for the reaction. The conversion of benzene is improved from less than 30% to 63% while the selectivity is kept at about 78%.										
Recovery of Cyclohexene										
US 5865958	Mitsubishi Chemical	10/20/95	Cyclohexene	--	--	--	--	--	--	
The reaction mixture of partial hydrogenation of benzene contains cyclohexene, cyclohexane, and unreacted benzene. Cyclohexene is recovered from this mixture by extractive distillation with 1,3-dimethyl-2-imidazolidinone serving as an extraction solvent. A series of four distillation columns is cited for the recovery.										
Adipic acid from Butadiene										
Hydrocarboxylation of Butadiene										
US 5962732	DuPont	12/17/98	Butadiene	Ni catalyst promoted with Aq. HI and 2,6-lutidine	115	6.9	5	98	82-88	
3-Pentenoic acid (3-PA) is prepared from butadiene by hydrocarboxylation in the presence of Ni catalyst with promoters, such as aqueous HI and 2,6-lutidine. Acetic acid serves as a solvent for the reaction. After 1 hr reaction, the conversion is 79 % with a selectivity of >90%. In the absence of water, butadiene can be carbonylated to 3-PA but the reaction is relatively slower.										

Table 4.4 (Continued)
TECHNOLOGY FOR ADIPIC ACID

PATENT SUMMARY										
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)	
Hydrocarboxylation of Butadiene (continued)										
US 6133477	DuPont	7/23/97	Butadiene	Rh catalyst promoted with Aq. HI	140	3.5	--	--	--	
3-PA is prepared from butadiene by reaction with CO and water in the presence of a Rh catalyst promoted with HI. An aliphatic acid, such as nonanoic acid and heptanoic acid, serves as a solvent. The reaction mixture is flashed to remove CO and unreacted butadiene, and is sent to a stripping column with CO as stripping gas at 135-155°C to recover 3-PA as an overhead. A large number of plates and a high reflux ratio is necessary for complete removal of Rh catalyst from the overhead.										
US 5250726	DuPont	8/24/92	Butadiene	A duel catalyst system of heterogeneous or homogeneous sulfonic acid and Rh catalyst promoted with Aq. HI	88	4.7	3-4	72-77	87-95	
Butadiene is hydrocarboxylated to 3-pentenoic acid in acetic acid in the presence of a duel catalyst system. The preferred catalyst system is a combination of macroporous and microporous ion exchange resin, such as Amberlyst RTM. 15, Amberlyst RTM. XN-1010, Amberlyst RTM. IR-118, and Amberlyst RTM. IR-120, and a Rh catalyst promoted with HI. The amount of water is 10-15 wt% based on the reaction mixture. The concentration of the Rh catalyst is 0.04-0.1 wt%.										
US 5166421	DuPont	3/18/91	Butadiene	Rh catalyst and HI promoter	200	4.2	2.0	>90	~87 ADA and Branched diacid	
ADA is prepared from butadiene by hydrocarboxylation in acetic acid in the presence of Rh catalyst and HI promoter [as Rh(CO) ₂ I ₂ complex and free HI]. The resulting reaction mixture contains 2-methyl glutaric acid, adipic acid, dimethylsuccinic acid, ethylsuccinic acid, valeric acid, and γ-valerolactone. The mixture is cooled to 60°C to crystallize and remove ADA. The supernatant is subjected to isomerization at 230°C and 6.2 MPa under syngas for 2 hr to convert 2-methyl glutaric acid to ADA. The yield to ADA reported in the example is not desirable.										
US 5145995	DuPont	6/26/89	Butadiene	Rh catalyst and HI promoter	150	4.9	2.0	90	87	
3-Pentenoic acid is prepared from butadiene in acetic acid as solvent in the presence of Rh catalyst and HI. The preferable molar ratio of I/Rh ranges from 1:1 to 6:1, that of butadiene/Rh ranges from 80:1 to 82:1. The initial molar ratio of water/butadiene ranges from 2.3:1 to 2.5:1. The high I/Rh ratios reduce the selectivity to 3-pentenoic acid and increase selectivities to methylglutaric acid and ADA. The catalyst died rather rapidly at the I/Rh ratio exceeding 6:1. The excess water/butadiene ratios also reduce selectivity to 3-pentenoic acid.										
US 5763655	R.P. Fiber and Resin Intermediates	4/20/95	Butadiene	Ir catalyst and a halide promoter	160	10.0	4.0	71	40-45 (yield)	
3-Pentenoic acid is prepared from butadiene in 3-pentenoic acid as solvent in the presence of Ir catalyst and a promoter selected from HI, HBr, methyl iodide, or methyl bromide. The molar ratio of iodine or bromine to Iridium ranges from 1:1 to 5:1. The amount of catalyst ranges from 10 ⁻⁴ to 10 ⁻¹ mol/l of the reaction mixture. The concentration of butadiene in the reaction mixture is preferably ≤ 5.5 wt%.										

Table 4.4 (Continued)
TECHNOLOGY FOR ADIPIC ACID

PATENT SUMMARY									
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Hydrocarboxylation of Butadiene (concluded)									
US 5625096	Rhone-Poulenc Chimie	10/19/93	Butadiene	Pd catalyst and crotyl chloride	140	20.0	0.5-1.2	78-92	89.5-95 (yield)
3-Pentenoic acid is prepared from butadiene in the presence of crotyl/Pd chloride π-complex and excess crotyl chloride as co-catalyst. The crotyl/Pd chloride π-complex is prepared from PdCl ₂ and crotyl chloride under CO. Other by-products are 2-methyl glutaric acid 2-ethylsuccinic acid, γ-valerolactone, and butene.									
Hydrocarboxylation of Pentenoic Acids									
US 5710325	DuPont	11/1/96	3-Pentenoic acid (3-PA)	Ir catalyst promoted with HBr or HI	180	2.8-	5	68.4	66.8
ADA is prepared from 3-PA or its isomers by hydrocarboxylation in the presence of γ-valerolactone and 2-methylglutaric acid at 60 wt% and 34 wt% of reaction mixture, respectively. A strong acid, such as phosphoric acid, can be optionally used as an additional promoter. In the presence of excess γ-valerolactone suppresses the conversion of pentenoic acid to γ-valerolactone thus promotes the yield of ADA., which is recovered from the mixture by crystallization at 20°C.									
US 5218144	DuPont	12/10/91	3-PA	Ir catalyst and HI promoter	170-190	3.5-4.9	1.3	--	60-71
ADA is prepared from 3-PA in acetic acid in the presence of an Ir catalyst and HI promoter. The molar ratio of iodide to iridium is about 2:1 –3:1. The concentration of the catalyst is 800-2000 ppm, and that of the promoter is 500-8000 ppm both based on the reaction mixture.									
US 5312979	Rhone-Poulenc Chimie	7/9/92	3-PA	Rh catalyst and HI promoter	175	0.8-2.0	1.5	38-47	49-62 (yield)
ADA is prepared from pentenoic acids in the presence of Rh catalyst in the absence of solvent. The molar ratio of pentenoic acid to water is greater than 4:1.									
US 5420346	Rhone-Poulenc Chimie	9/29/92	3-PA	Ir catalyst and HI promoter	170	2.0	>0.5	95-100	63-75 (yield)
ADA is prepared from 3-PA by reacting with water and CO in a solvent in the presence of Ir catalyst (Ir ₄ (CO) ₁₂) and HI as a promoter. The Ir catalyst is Ir ₂ (CO) ₁₂ , or Ir(AcAc)(CO) ₂ with an I/Ir molar ratio preferably ranging from 1:1 to 5:1. The solvents include toluene, chlorobenzene, methylene chloride, 1,2-dichloroethane and diphenyl ether.									
US 5227522	Rhone-Poulenc Chimie	4/26/91	3-PA	Ir catalyst and HI promoter	175	2.0	1/3	60-95	59-77
ADA is prepared from pentenoic acid by reacting with water and CO in the presence of Ir-based catalyst and HI as a promoter. An aliphatic acid, such as acetic acid 3-PA or ADA can be used as a solvent. The molar ratio of I/Ir ranges from 1:1 to 5:1. That of water to pentenoic acid ranges from 0.01:1 to 10.0:1. When ADA is used as solvent for the reaction the conversion is increased to 95% and selectivity to ADA at 77%.									

Table 4.4 (Continued)
TECHNOLOGY FOR ADIPIC ACID

PATENT SUMMARY									
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Hydrocarboxylation of Pentenoic Acids (concluded)									
US 5268505	Rhone-Poulenc Chimie	12/20/90	3-PA	Rh catalyst, cocatalyst, and HI promoter	175	1.0	1-1.5	92-100	50-69 (yield)
3-Pentenoic acid is hydrocarboxylated in the presence of Rh catalyst, a cocatalyst and HI as a promoter. The cocatalysts include IrCl ₃ , RuCl ₃ , OsCl ₃ , and IrCl ₃ . The molar ratio of the metal in the cocatalyst to Rh ranges from 0.1 to 5.0. The molar ratio of I/Rh ranges from 1 to 10. The concentration of Rh ranges from 10 ⁻³ to 10 ⁻¹ mol/l.									
US 5227523	Rhone-Poulenc Chimie	9/28/90	Pentenoic acids	Rh catalyst, cocatalyst, and HI	175-190	1.2	≤1.0	62-100	36-69 (yield)
Hydrocarboxylation is conducted in the presence of a solvent selected from aliphatic or aromatic hydrocarbons, or chlorinated derivatives thereof. 4-pentenoic acid provides the highest yield among the pentenoic acids, while 2-pentenoic acid gives the lowest.									
US 5198577	Rhone-Poulenc Chimie	9/18/90	3-PA	Rh catalyst, and HI promoter	175	0.8-1.5	20-30 min	100	54-72
3-PA is hydrocarboxylated in acetic acid in the presence of Rh catalyst, and HI as a promoter. The concentration of the Rh catalyst ranges from 5x10 ⁻³ to 3x10 ⁻¹ mol Rh/l of reaction mixture. The I/Rh molar ratio ranges from 1:1 to 4:1									
US 5359137	DuPont	4/26/89	γ-Valerolactone or α-methylbutyrolactone	Rh catalyst and HI promoter	200 or 220	4.2 or 8.0	4 or 5	78-80 or 78-100	67 or 15-26
ADA is prepared from γ-valerolactone or α-methylbutyrolactone by hydrocarboxylation in the presence of a homogeneous rhodium catalyst and HI as a promoter. The molar ratio of Rh/HI is from 1:1 to 1:20. Other by-products are methyl glutaric acid, ethylsuccinic acid, valeric acid, and dimethylsuccinic acid.									
Adipic acid from Cyclohexane									
Oxidation of Cyclohexane or Cyclohexanol									
US 6008415 US 5780683	ABB Lummus	9/11/96	Cyclohexane	Co naphthenate	149	0.9	8.0 min.	5	78
Cyclohexane is oxidized in a series of 3-4 reactors with oxygen-enriched air (30-90 vol%) or pure oxygen to improve the selectivity to KA oil over a shorter residence time. The reactor is equipped with a hollow shaft chamber, and helical impeller means, which is positioned inside the chamber and provide a downward flow of the reaction mixture through the chamber and upward flow through the annular area between the reactor wall and the outside wall of the hollow chamber. A baffle with a number of opening is positioned a short distance below the gas-liquid interface to keep most oxygen bubbles within the main reaction body with the help of attached guide baffle means. To keep the oxygen concentration in the gas phase above the gas-liquid interface below the flammability limit, inert gas let means are provided below and above the perforated baffle. The oxygen-enriched air is fed to a lower position inside the hollow chamber. The reaction product is stripped with nitrogen to remove oxygen followed by hydrogenation to convert some of cyclohexyl hydroperoxide (CHHP) to KA oil before recovery of cyclohexanol and cyclohexanone by distillation.									
JK 09077705	Daicel Chemical	9/13/95	Cyclohexanol	Redox agents	20-40	Autogenous	1-2	80-99	80-100
An aqueous solution of cyclohexanol and NaBrO ₃ is mixed with equal volume of acetonitrile. The resulting solution is slowly added to an aqueous solution of sodium hydrogen bisulfite. The amount of the oxidizing agent is 1.2-1.4 moles per mole of cyclohexanol. The molar ratio of the reducing agent to the oxidizing agent is 1.0:1.0.									

Table 4.4 (Continued)
TECHNOLOGY FOR ADIPIC ACID

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Oxidation of Cyclohexane or Cyclohexanol (concluded)									
US 6160183	DuPont	2/10/98	Cyclohexane	Au catalyst supported on alumina and sol-gel compounds	160-170	3.5	36-39 min	3.2-4.9	98.6-92.3
Cyclohexane is oxidized directly to KA oil with little or no formation of CHHP in the reaction mixture so that the conventional operation step of decomposing CHHP can be omitted. The reaction is carried out in a small glass vial as cited in the examples. The sol-gel compounds include AuMgCrAlO, AuMgCrZrO and others.									
US 6147256	Rhodia Fiber and Resin Intermediates	4/10/97	Cyclohexane	Co-acetate(H ₂ O) ₄ and Cr-acetate	105 105	10 10	1.0 1.9	12.2 15.0	67.3 79.5
Cyclohexane is oxidized in acetic acid in the presence of small amount of cyclohexanone and a catalyst of cobalt acetate and chromium acetate. The reaction is carried out in a titanium autoclave with a heating collar and turbomixer.									
Decomposition of Cyclohexyl Hydroperoxide									
US 5959153	DSM	3/12/97	Cyclohexyl hydroperoxide	Co catalyst on TiO ₂	62	Atmospheric	--	--	>92
A cyclohexane oxidation mixture, containing CHHP, is subjected to decomposition at 62°C in the presence of methanol, ethanol or 1-propanol, and an aqueous solution of NaOH and Na ₂ CO ₃ .									
US 5905173	DSM	10/13/95	Cyclohexyl hydroperoxide	CoSO ₄ and/or Na-acetate	66-90	Atmospheric	--	> 95	--
A cyclohexane oxidation mixture, containing CHHP, is subjected to decomposition at 66-90°C in the presence of an aqueous solution of NaOH and Na ₂ CO ₃ .									
US 5859301	DSM	12/23/93	Cyclohexyl hydroperoxide	Co catalyst on TiO ₂	73	Atmospheric	--	--	~100
A cyclohexane oxidation mixture, containing CHHP, is subjected to decomposition at 73°C in the presence of an aqueous solution of Na ₂ CO ₃ , K ₂ CO ₃ or NaOH. Other catalysts include Ni, Cu, Fe, and Mn supported on TiO ₂ . The molar ratio of cyclohexanol to cyclohexanone is 0.64-0.74:1. The reaction rate reportedly ranges from 10x10 ⁻⁴ to 46x10 ⁻⁴ kg solution/g cat./min.									
US 5892122	DuPont	8/25/97	Cyclohexyl hydroperoxide	Co catalyst	--	--	--	--	--
A cyclohexane oxidation mixture, containing CHHP, is subjected to decomposition at 66-90°C in the presence of an aqueous caustic solution, such as NaOH, NaHCO ₃ and Na ₂ CO ₃ . After phase separation, the organic phase, containing KA oil is extracted with water along with a polyprotic acid to neutralize the residual caustic to a pH of 7-9.5 to avoid oligomerization of cyclohexanone during purification by distillation.									
US 6284927	DuPont	4/30/97	Cyclohexyl hydroperoxide	A heterogenous catalyst of Au, Ag, or Cu	125-150	Atmospheric	5-10	45-71	~100
A mixture, containing CHHP and KA oil, is subjected to decomposition at 125-150°C in the presence of the heterogenous catalyst. A sol-gel compound, such as CrZrO, CrTaO, CrTiO, or CoCrTiO, can also be used to catalyze the decomposition reportedly with higher conversion up to 93-100%.									

Table 4.4 (Continued)
TECHNOLOGY FOR ADIPIC ACID

PATENT SUMMARY									
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Decomposition of Cyclohexyl Hydroperoxide (concluded)									
US 6191311	DuPont	4/30/97	Cyclohexyl hydroperoxide	Catalyst of Ti, Zr, or Nb, supported on silica	115-125	Atmospheric	5-10 min	38-87	~100
A mixture, containing CHHP and KA oil, is subjected to decomposition at 125-150°C in the presence of the heterogenous catalyst. Other sol-gel compounds, such as ZrSiO and TiSiO, can also be used as the heterogenous catalyst.									
Direct Oxidation of Cyclohexane									
US 5900506	R.P. Fiber and Resin Intermediates	12/12/96	Cyclohexane	Co-acetate·4H ₂ O	105	2.0	~1.5	20	58.9
Cyclohexane is directly oxidized to ADA in acetic acid in the presence of small amount of cyclohexanone and the Co catalyst. The reaction is carried out in a titanium autoclave with a heating jacket and a six paddle turbomixer. The reaction mixture is decanted at 70°C to separate an upper cyclohexane phase and a lower acetic acid phase. After separation, the acetic acid phase is subjected to distillation under 135°C and 0.03-0.045 MPa to remove acetic acid, cyclohexanol and cyclohexanone along with less amounts of cyclohexyl acetate, butyrolactone and valerolactone. The distillation residue contains mainly ADA along with dibasic acids and hydroxyl monobasic acids. The distillate accounts for about 86 wt% of the acetic acid phase. The remaining residue is mixed with water and then cooled gradually to room temperature to crystallize ADA.									
US 5756837	Rhone-Poulenc Fiber & Resin Intermediates	7/13/95	Cyclohexane	Co-acetate·4H ₂ O	106-107	2.0	125-130 min.	20-24	68 to ADA 14-15 to KA oil
ADA is prepared by direct oxidation of cyclohexane in the presence of a Co catalyst, with acetic acid as a solvent, and acetaldehyde as an initiator. A depleted air (5.85% oxygen) is initially used for the reaction. The oxygen content of the depleted air is increased to 11.35% when the oxygen content of the air, leaving at the reactor outlet, reaches to 1%. After the reaction, the mixture is first gradually cooled to 75°C and then rapidly cooled to 20°C to precipitate ADA. After the removal of the solid phase, the resulting liquid is settled into an acetic phase and cyclohexane phase. The acetic phase is concentrated at 50°C and 4 kPa to remove water, and some of the acetic acid, cyclohexane, and KA oil. The concentrated acetic phase is then extracted with cyclohexane to precipitate the Co catalyst, which is recycled to the oxidation reactor along with fresh Co catalyst, cyclohexane, and acetic acid. The supernatant liquid can be distilled to separate KA oil from the by-products. All the recovered KA oil, acetic acid, and cyclohexane can be recycled to the oxidation reactor.									
Purification of Adipic Acid									
US 5210297	BASF	12/30/91	--	--	--	--	--	--	--
ADA is prepared by oxidation of KA oil (a mixture of cyclohexanone and cyclohexanol) with nitric acid in the presence of Cu and V catalysts. ADA thus produced is recovered by crystallization. Typically, a mother liquor from crystallization contains 30-36 wt% nitric acid, 15-21 wt% water, 10-13 wt% succinic acid, 23-30 wt% glutaric acid, 9-11 wt% ADA, 0.7-0.8 wt% Cu, 0.08-0.09 wt% V, 0.002-0.004 wt% Fe, and other impurities, such as nitrogen compounds. The mother liquor is distilled to remove nitric acid as an azeotrope with water under reduced pressure. The resulting melt is heated to 150-160°C and 150-950 mbar to decompose nitrogen compounds and oxalic acid, and dissolved in water. The resulting aqueous solution is treated with cation exchange resin to separate Cu and V ions before it is subjected to evaporation to remove the water, and distillation to obtain a mixture of dicarboxylic acids, which are suitable to prepare polyesterpolymers.									
US 5587511	Bayer	11/18/94	--	--	--	--	--	--	--
The mother liquor from ADA crystallization contains glutaric acid and succinic acid along with ADA in an aqueous HNO ₃ solution. There were several ways to convert both glutaric acid and succinic acid to imides amides or esters before the by-products are separated from ADA, but they are not satisfactory. The present method is to evaporate nitric acid and water from the mother liquor down to a residual content of < 2.5 wt%. The concentrate is then mixed with either water or dilute nitric acid so that the weight ratio of solids to liquid is 1:1.8 to 1:1.3. The mixture is agitated at 70°C for 5-10 minutes. The mixture is cooled to 35°C over a period of 90 minutes to isolate the acid crystals, which is separated by filtration and contains about 80-90 wt% ADA. The yield of ADA is 70-75%.									

Table 4.4 (Continued)
TECHNOLOGY FOR ADIPIC ACID

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Purification of Adipic Acid (continued)									
DE 4440916	Bayer	11/17/94	--	--	--	--	--	--	--
Crude ADA (20 wt% in water) from oxidation of cyclohexane is purified by extraction with MIBK, to reduce Co content in the crude ADA from 1000 mg/kg to 0.1 mg/kg. The resulting ADA in MIBK solution is further extracted with water to reduce organic impurities to below 1 wt%. Extracted ADA is crystallized to produce purified ADA.									
DE 4440733	Bayer	11/15/94	--	--	--	--	--	--	--
Crude ADA from oxidation of cyclohexane is purified by extraction with a hydrophobic solvent, cyclohexane, to remove monocyclohexyl adipate. The resulting solution is further extracted with 12 wt% aqueous sulfuric acid. Extracted ADA is washed with water and crystallized to produce purified ADA containing 0.4 mg/kg Co catalyst.									
US 5481033	DuPont	12/22/94	Branched dicarboxylic acids	Ir catalyst and HI	210-230	2.8	4-24	7.4-84-	1-6.8 (yield)
ADA is separated by crystallization from a reaction mixture obtained by hydrocarboxylation of pentenoic acid. The resulting mixture of by-products is isomerized in the presence of Ir catalyst along with HI as a promoter.									
US 5292944	DuPont	6/29/93	Branched dicarboxylic acids	Ir catalyst and HI	210-230	2.8	4-24	7.4-84-	1-6.8 (yield)
ADA is separated by crystallization from a reaction mixture obtained by hydrocarboxylation of pentenoic acid. The resulting mixture of by-products is isomerized in the presence of Ir catalyst along with HI as a promoter.									
WO 00/15597 WO 99/44980	Rhodia Fiber & Resin Intermediates	9/14/98 3/5/98	--	--	--	--	--	--	--
ADA is prepared by direct catalytic oxidation of cyclohexane in an organic solvent. The reaction mixture is decanted into an upper phase, which consists predominantly of unconverted cyclohexane. The lower phase consists of ADA, the catalyst, other by-products and some cyclohexane in solvent. The lower phase is distilled to remove the solvent along with unconverted cyclohexane and other volatile components as overhead distillate. The bottom stream is washed with water followed by crystallization to obtain purified ADA.									
US 6222069 WO 97/465510 WO 97/465509	Rhone-Poulenc Fiber & Resin Intermediates	6/4/96	--	--	--	--	--	--	--
ADA is prepared by either direct oxidation of cyclohexane in the presence of Co catalyst or by hydrocarboxylation of 3-pentenoic acid in the presence of Rh or Ir catalyst. After preliminary purification, the ADA containing traces of catalyst is further purified by crystallization in the presence of a strong acid and/or carbon monoxide to reduce the Co catalyst content to 0.00009 wt%, or Rh (or Ir) catalyst to 0.0005 wt%. The strong acid can be HI, HBr, HCl, or sulfuric acid. The molar ratio of acid to catalyst in the ADA is 10:1, and CO pressure ranges from 1 to 50 bars.									

4.4 (Concluded)
TECHNOLOGY FOR ADIPIC ACID

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Purification of Adipic Acid (concluded)									
US 5756837	Rhone-Poulenc Fiber & Resin Intermediates	7/13/95	Cyclohexane	Co-acetate·4H ₂ O	106-107	2.0	125-130 min.	20-24	68 to ADA 14-15 to KA oil

ADA is prepared by direct oxidation of cyclohexane in the presence of a Co catalyst, with acetic acid as a solvent, and acetaldehyde as an initiator. A depleted air (5.85% oxygen) is initially used for the reaction. The oxygen content of the depleted air is increased to 11.35% when the oxygen content of the air, leaving at the reactor outlet, reaches to 1%. After the reaction, the mixture is first gradually cooled to 75°C and then rapidly cooled to 20°C to precipitate ADA. After the removal of the solid phase, the resulting liquid is settled into an acetic phase and cyclohexane phase. The acetic phase is concentrated at 50°C and 4 kPa to remove water, and some of the acetic acid, cyclohexane, and KA oil. The concentrated acetic phase is then extracted with cyclohexane to precipitate the Co catalyst, which is recycled to the oxidation reactor along with fresh Co catalyst, cyclohexane, and acetic acid. The supernatant liquid can be distilled to separate KA oil from the by-products. All the recovered KA oil, acetic acid, and cyclohexane can be recycled to the oxidation reactor.

US 5587056	Rhone-Poulenc Chimie	6/14/94	--	--	--	--	--	--	--
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Separation of branched diacidic compounds, such as 2-methylgluatic acid and 2-ethylsuccinic acid, from adipic acid in a mixture of these compounds is carried out first by anhydriization of these branched dicarboxylic acids followed by distillation of the resulting mixture. The mixture may originate from the recovery of the diacids in aqueous phases of recrystallization of ADA, or from the diacid distillation residue. The anhydriization is carried out at 120°C in the presence of a homogeneous catalyst, such as concentrated sulfuric acid or para-toluenesulfonic acid, or a heterogeneous catalyst, such as boron phosphate or montmorillonite acidic clay.

JK 11267405	Ube Industries	3/20/98	--	--	--	--	--	--	--
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Reaction mixture from oxidation of cyclohexane is used with 80°C hot water through a static mixer. The resulting mixture is phase-separated with a liquid cyclone settler. About 75% of ADA is extracted into the aqueous phase without forming scale inside the settler.

Treatment of Nitrogen Oxide

US 6056928	BASF.	9/12/95	N ₂ O	Ammonium mordenite	500-540	--	--	--	--
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In the oxidation of KA oil with nitric acid, the reaction produces nitrogen oxides as a waste gas, which typically comprises 20 vol% NO₂, 23 vol% N₂O, 10 vol% O₂, 2 vol% carbon oxides, and the remainder of nitrogen and some inert gas, such as Ar. The gas mixture is initially subjected to absorption at 30-40°C with water or dilute nitric acid in the presence of free oxygen to remove nitrogen oxides other than dinitrogen oxide. The gas stream from the absorption is heated to 450-500°C before it is catalytically reduced with ammonia to nitrogen and water. Other catalysts can be zeolites, which have been exchanged metals, such as Fe, Co, Cu, Rh, Pd, or Ir.

US 5582810	Grande Paroisse S.A.	5/10/93	N ₂ O	Ammonium mordenite	500-540	--	--	--	--
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The nitrous oxide in the gaseous effluent from ADA production is catalytically decomposed at 500-540°C in the presence of ammonium mordenite, which is prepared from ammonium nitrate and small-pore sodium mordenite having a formula of Na₇(AlO₂)₇(SiO₂)₄₀·24H₂O. It is preferred that the catalyst has been exchanged with iron or cobalt. It is desirable to add nitrogen oxides (NO and NO₂) when the nitrous oxide concentration in the gas effluent is 20-30 wt%.

Table 4.5
TECHNOLOGY FOR HEXAMETHYLENEDIAMINE

PATENT SUMMARY									
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Hydrocyanation of Butadiene									
WO 99/64155	BASF	6/5/98	1,3-butadiene	Ni(COD)2 and bidentate phosphonite ligand	70-90	0.12	2.0	99	99.4 3PN, 4PN and 2M3BN
New catalysts comprises complexes of Group VIII metal (e.g. Ni(COD)2, where COD is 1,5-cyclooctadiene) and a bidentate phosphonite ligand with alkylene bridge. The catalysts are used for hydrocyanation of butadiene for adiponitrile production, or for isomerization of aliphatic monoalkenenitrile. The ligands are prepared from (C6H5)PCl2, 1,1'-binaphthol and substituted phenol. The molar ratio of 3-pentenenitrile (3PN) to 2-methyl-3-butenenitrile (2M3BN) is 0.22:1-0.41:1. The same catalyst system can be used for isomerization of 2M3BN to 3PN at 110°C. The molar ratio of 3PN to 2M3BN is increased to 4.75:1 after 6 hours of reaction, and to 8.25:1 after 22 hours.									
US 6169198	BASF	8/4/97	1,3-butadiene	Ni(COD)2 and 1,1'-bis(diphenyl-phosphino)-ferrocene	80-90	0.14-0.34	3.2-4.0	99-100 based on HCN	81-84.7 3PN and 2M3BN
An Ni(0) complexed with a ferrocene-phosphine compound is used as catalyst system for the hydrocyanation of 1,3-butadiene or C4 cut (40 vol% 1,3-butadiene, 30 vol% isobutene, and 14.3 vol% 1-butene) in toluene. The molar ratio of 3PN to 2M3BN is 23.8:1-30:1.									
US 6171997 US 6120700	DuPont	7/29/97	1,3-butadiene	Ni(COD)2, multidentate phosphite ligand	80	--	1.5	62.3-83.6	>99 3PN and 2M3BN
			2-methyl-3-butenenitrile		125	--	1.5	92.3-94.2	93.7-95.1 3PN yield
PCl3 reacts with bulky ortho-substituted phenols in the presence of triethylamine (TEA) to form phosphorochloridites, which are further reacted with various aromatic dihydroxy compounds in the presence of TEA to form various multidentate phosphite ligands. These phosphite ligands are combined with Ni(0), such as Ni(COD)2, to form various "catalyst precursor compositions". The catalyst composition is referred to, as a "precursor" here only to indicate in all likelihood, during the hydrocyanation reaction the structure of the active catalyst composition may in fact be complexed to an olefin. The catalyst compositions are used for hydrocyanation of butadiene or isomerization of 2-methyl-3-butenenitrile (2M3BN). The catalyst compositions, having ligands with bulky substituted aromatic groups, provides higher conversion in either hydrocyanation or isomerization reaction with higher selectivities to PNs.									
US 6121184	DuPont	7/29/97	1,3-Butadiene	Ni(COD)2, and a supported bis(phosphorus) ligand	80	--	1.5-3.0	12-40	--
Various resin supported diols are used to react with bis(phosphorus) compounds to produce resin supported ligand, which is combined with Ni(COD)2 to form catalyst systems for the hydrocyanation of butadiene or 3-PN. The molar ratio of 3PN to 2M3BN ranges from 0.67:1 to 1.72:1. The same catalyst system can be used for gas-phase hydrocyanation at 145°C over a period of 3 hours with 87-100% selectivity to a mixture of 3PN and 2M3BN.									
US 5693843	DuPont	12/22/95	1,3-Butadiene	Ni(COD)2, bidentate phosphorus ligand	80	Autogenous	1-3.0	30-100	21-36% to 3-PN 31-71% to 2M3BN
The bidentate diphosphinites are prepared by reacting diarylchlorophosphine, such as diphenylchlorophosphine, with an aromatic diol, such as 1,1'-binaphthol, and triethylamine in toluene solution. The reaction mixture is stirred at room temperature. After the reaction, the mixture is filtered to remove triethylamine hydrochloride. The resulting bidentate phosphorus ligand is recovered by removing the solvent under reduced pressure. Ni(COD)2 is then complex with the ligand to form the desired catalyst for hydrocyanation of butadiene or isomerization of 2M3BN in propionitrile.									

Table 4.5 (Continued)
TECHNOLOGY FOR HEXAMETHYLENEDIAMINE

PATENT SUMMARY									
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Hydrocyanation of Butadiene (continued)									
US 5821378	DuPont	11/28/95	1,3-Butadiene	Ni(COD)2 and multidentate phosphite ligand	80	--	3.0	89-98	73-76 to 2M3BN 18-19 to 3PN (Yield)
			2M3BN		125	Atmospheric	3.0	93-95	86-96 (yield)
The multidentate phosphite ligand is prepared by reacting PCl_3 with 2,2'-biphenol to give 1,1'-biphenyl-2,2'-dyl phosphorochloridite, which is further reacted with 2,2'-dihydroxy-3,3'-di-t-butyl-5,5'-dimethoxy-1,1'-biphenyl. The catalyst composition is used for either hydrocyanation of butadiene or isomerization of 2M3 to 3-PN and/or 4-PN.									
US 5696280	DuPont	1/27/95	1,3-Butadiene	Ni(COD)2 and multidentate phosphite ligand	80 or 140	Autogenous	1.0	88-98	17-32 to 3-PN 63-77 to 2M3BN
The phosphite ligands having multidentate groups are prepared from PCl_3 , 2,2'-biphenol, and a third dihydroxy aromatic compound, such as 2,2'-dihydroxy-3,3'-di-t-butyl-5,5'-dimethoxy-1,1'-biphenyl. The 2M3BN is isomerized at 125°C for 3 hr to 3-PN in the presence of same catalyst system with >94% conversion and >99% selectivity.									
US 5449807	DuPont	11/18/94	1,3-Butadiene	Supported Ni(0) and bidentate phosphite ligand	150	Autogenous	?	100 (HCN)	>76 to 3PN
1,3-Butadiene is converted to 3-PN by gas-phase hydrocyanation in the presence of a silica supported Ni catalyst and bidentate phosphite ligand.									
Isomerization of 2-Methyl-3-Butenenitrile									
US 5440067	DuPont	11/18/94	2M3BN	Supported Ni(0) bidentate phosphite ligand	145-150	Autogenous	?	91-92	77-78
2M3BN is converted to 3-PN by gas-phase isomerization in the presence of a silica supported Ni catalyst.									
US 5486643	Rhone Poulenc Chimie	10/8/93	2M3BN	Ni(COD)2 and TSTPP	90	Autogenous	1.5	87-95	91-94
2M3BN is isomerized to 3-PN in the presence of the Ni(0) catalysts. TSTPP is sodium salt of trisulfonated triphenylphosphine.									
US 5834616	Rhone-Poulenc Fiber & Resin Intermediates	12/12/95	2-Methylglutarimide	Acidic zeolite with $\text{SiO}_2/\text{Al}_2\text{O}_3 = 51:1$ to 350:1	250-500	0.01-5.0	0.8-1.6 seconds contact time	89-99	67-77
2-Methylglutarimide and/or ethylsuccinimide are converted to pentenenitriles in the presence of acetonitrile as a solvent. The distribution of 2-PN:3-PN:4-PN is 28-41:53-44:19-15.									

Table 4.5 (Continued)
TECHNOLOGY FOR HEXAMETHYLENEDIAMINE
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Hydrocyanation of Pentenenitrile									
US 6048996	DuPont	8/26/99	3-Pentenenitrile and/or 4-pentenenitrile	Ni(0), (m,p-TTP)4 ligand and an insoluble promoter	60-70	--	1.0	50-73	90-94
Ni(0) is complexed with (m,p-TTP)4 ligand, which is used the production of ADN by the hydrocyanation of 3-pentenenitrile (3-PN) and/or 4-pentenenitrile (4-PN) in the presence of an insoluble promoter selected from metal oxides, such as Fe ₂ O ₃ , Fe ₃ PO ₄ , TiO ₂ and ZnO; and metal halides, sulfates, and phosphates. The m,p-TTP refers to meta and para tritylphosphite, and it is used in excess amounts in respective to Ni(0). The use of insoluble promoter provides easy separation from the reaction mixture by filtration.									
US 6171996	DuPont	7/13/99	3-PN	Ni(COD) ₂ , multidentate phosphite ligand and ZnCl ₂	70	--	1.0	56-95	85-93
PCl ₃ reacts with 2-alkylophenol, such as o-cresol, 2-ethylphenol or 2-n-propylphenol, in the presence of triethylamine (TEA) to form phosphorochloridites, which are further reacted with various aromatic dihydroxy compounds, such as 1,1'-binaphthol, 2,2'-biphenol, and in the presence of TEA to form various multidentate phosphite ligands. These phosphite ligands are combined with Ni(0), such as Ni(COD) ₂ , to form various "catalyst precursor compositions". The catalyst composition is referred to as a "precursor" here only to indicate in all likelihood, during the hydrocyanation reaction the structure of the active catalyst composition may in fact be complexed to an olefin. The catalyst compositions are used for hydrocyanation of 3-PN. The catalyst compositions, having ligands with carboxylate- or alkoxy-substituted bulky aromatic groups, provide relatively lower conversion of 3-PN, and those with less bulky groups provide relatively lower selectivities to ADN.									
US 5959135	DuPont	7/8/98	3-PN	Ni(COD) ₂ , multidentate phosphite ligand and ZnCl ₂	70	?	1.0	33-88	76-91
3-PN is hydrocyanated with HCN under nitrogen in the presence of a nickel catalyst system. The multidentate phosphite ligands are prepared by reacting PCl ₃ first with 1-naphthol or 4-methoxy-1-naphthol in the presence of TEA, toluene and THF to form phosphorochloridite, which is then reacted with a third dihydroxy aromatic compound selected from 2,2'-binaphthol, 3,3'-dimethoxy-5,5'-di-2-propenyl-2,2'-dihydroxy-1,1'-biphenylene, 2,2'-dihydroxy-3,3'-dimethoxy-5,5'-dimethyl-1,1'-biphenylene, and dimethyl 2,2'-dihydroxy-1,1'-binaphthalene-3,3'-dicarboxylate. As reported in US 6171996, the catalyst compositions, having ligands with carboxylate substituted bulky aromatic groups, provide relatively lower conversion of 3-PN, and those with less bulky groups provide relatively lower selectivities to ADN.									
US 6127567 US 6020516 US 5981772 US 5847191	DuPont	7/29/97	3-PN	Ni(COD) ₂ , multidentate phosphite ligand and ZnCl ₂	70	< 1.0	1.0	64-95	84-95
3-PN is hydrocyanated with HCN under nitrogen in the presence of a nickel catalyst system. The Ni catalyst precursor is Ni(COD) ₂ . The phosphite ligands having multidentate groups are prepared from PCl ₃ , 2-alkylophenol, and a third dihydroxy aromatic compound selected from 1,1'-binaphthol, 2,2'-dihydroxy-1,1'-biphenylene, 2,2'-biphenol compound or their substituted derivatives.									
US 5723641 US 5688986	DuPont	9/26/96 11/7/94	3-PN	Ni(COD) ₂ , bidentate phosphite ligand and ZnCl ₂	50-70	?	2.0	26-68	71-95
The bidentate phosphite ligand is prepared first by reacting excess PCl ₃ with 2,2'-biphenol to form 1,1'-biphenyl-2,2'-dyl phosphorochloridite. The excess PCl ₃ is removed by distillation. The phosphorochloridite is purified by vacuum distillation, and is then further reacted with 2,2'-dihydroxy-3,3'-di-t-butyl-5,5'-dimethoxy-1,1'-biphenyl in the presence of TEA and toluene. Other promoters can be ZnBr ₂ , ZnI ₂ , SnCl ₂ and BPh ₃ .									

Table 4.5 (Continued)
TECHNOLOGY FOR HEXAMETHYLENEDIAMINE

PATENT SUMMARY									
Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Hydrocyanation of Pentenenitrile (continued)									
US 5663369 US 5512696	DuPont	10/16/95 7/21/95	3-PN	Ni(COD) ₂ , multidentate phosphite ligand and ZnCl ₂	70	Autogenous	1-2	34-83	76-91
3-Pentenenitrile (3-PN) is hydrocyanated with HCN under nitrogen in the presence of a nickel catalyst system. The Ni catalyst precursor is Ni(COD) ₂ . The phosphite ligands having multidentate groups are prepared from PCl ₃ , 2-isopropylphenol, and a third dihydroxy aromatic compound selected from 1,1'-binaphthol, 2,2'-dihydroxy-1,1'-biphenylene, 2,2'-biphenol compound or their substituted derivatives.									
US 5523453	DuPont	3/22/95	3-PN	Ni(COD) ₂ , bidentate phosphite ligand and ZnCl ₂	70	Autogenous	1.0	50-68	74-97
The bidentate diphosphinites are prepared by reacting diarylchlorophosphine, such as diphenylchlorophosphine, with an aromatic diol, such as 1,1'-binaphthol, and triethylamine in toluene solution. The reaction mixture is stirred at room temperature for 1 hr. After the reaction, the mixture is filtered to remove triethylamine hydrochloride. The resulting filtrate is washed with toluene, and the bidentate phosphorus ligand is recovered by removing the solvent under reduced pressure. The molar ratio of bidentate phosphorus compound to nickel is 3:1, and that of nickel to ZnCl ₂ (a Lewis acid promoter) is 1:1. Other Lewis acids can be MnCl ₂ , FeCl ₂ , AlCl ₂ (C ₈ H ₁₇), and Ph ₃ Sn(Ph ₃ BCN).									
US 5543536	DuPont	4/26/94	3-PN	Ni(COD) ₂ , monodentate phosphite ligand and ZnCl ₂	70	?	2.0	56-71	82-86
The monodentate phosphite ligand is prepared by reacting PCl ₃ with either 2,2'-biphenol or 2-t-butyl-4-methoxyphenol to form 1,1'-biphenyl-2,2'-diyl phosphorochloridite or 2-t-butyl-4-methoxyphenyl phosphorodichloridite. The monochloride reacts further with 2-t-butyl-4-methoxyphenol, while the dichloride reacts with 2,2'-biphenol. In both cases, the reaction takes place in the presence of TEA and a solvent of toluene or THF. The monodentate phosphite ligand thus prepared is combined with Ni(0) and ZnCl ₂ to form a catalyst composition for hydrocyanation of 3-PN. Other dihydroxy aromatic compounds used are 2,2'-dihydroxy-5,5'-dimethoxy-1,1'-biphenyl, and 1,1'-bi-2-naphthol. Other monohydroxy aromatic compounds are 2-t-butylphenol, and 2-t-butyl-4-methylphenol.									
US 5512695	DuPont	4/14/94	3-PN	Ni(COD) ₂ , unsymmetrical bidentate phosphite ligand and ZnCl ₂	50-100	?	1.0-1.25	?	79-82
The unsymmetrical bidentate is prepared first by reaction of PCl ₃ with 2,2'-biphenol to form 1,1'-biphenyl-2,2'-diyl phosphorochloridite, which is further reacted with 2,2'-dihydroxy-3,3'-di-t-butyl-5,5'-dialkoxy-1,1'-biphenyl. The reaction is carried out in the presence of triethylamine and THF. After the reaction, the mixture is filtered to remove triethylamine hydrochloride. The resulting bidentate phosphorus ligand is washed and recovered by removing the solvent under reduced pressure. The unsymmetrical bidentate ligand thus prepared is combined with Ni(COD) ₂ and ZnCl ₂ , serving as a catalyst for hydrocyanation of 3-PN to ADN.									
US 4990645	DuPont	6/27/90	3-PN	Ni(0) catalyst and triaylborane	--	--	--	--	--
An improved process for the hydrocyanation of pentenenitriles is cited. It is to control HCN concentration in the product stream at < 2500 ppm, and to recycle part of solid catalyst degradation precipitate to the hydrocyanation reactor in order to minimize the fouling of process equipment caused by solid catalyst degradation precipitate. In the process, the reaction effluent is subjected to flashing to remove unconverted pentenenitriles. The crude ADN is then decanted with part of the lower phase, which contains solid catalyst degradation precipitate, is recycled to the hydrocyanation reactor. The remainder is discarded after washing with PN to recover the retained catalyst. The upper phase from the decanter is extracted with an organic solvent to remove the catalyst and ligand from ADN product. The catalyst in the extract is then separated from the solvent and recycled to the reactor.									

Table 4.5 (Continued)
TECHNOLOGY FOR HEXAMETHYLENEDIAMINE
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Hydrocyanation of Pentenenitrile (continued)									
EP 336314	DuPont	3/31/88	3-PN	Ni(0) catalyst and promoters	60	?	80	70-85	2.0
The Ni(0) catalyst is Ni(m,p-TTP)4, where m,p-TTP is a mixture of meta and para tolyl groups complexed with the Ni(0) metal. The promoters are BPh3 and one of Ph3SnO3SCF3, Ph3SnPh3BCN, and Cy3SnO3SCF3. The reaction involves isomerization of 3-PN to 4-pentenenitrile (4PN), and hydrocyanation of 4-PN to adiponitrile (ADN).									
US 5908805	Rhone-Poulenc Fiber & Resin Intermediates	12/29/95	--	--	--	--	--	--	--
An Ni[0] catalyst is prepared from Ni(CN)2 by hydrogenation in the presence of a water soluble phosphine compound, a supported Pd catalyst or supported Pt catalyst, and a Lewis acid, such as ZnCl2. The phosphine compound is sodium triphenylphosphine trisulfonate. The resulting catalyst system is used for hydrocyanation of 3-PN.									
US 5856555	Rhone-Poulenc Fiber & Resin Intermediates	9/29/95	3-PN	Ni(COD)2, Sulfonated triphenylphosphine and ZnCl2	60	--	0.5-0.75	7-19	69-81 to ADN, (yield)
The sulfonated phosphine ligands are water soluble, such as sodium salts of 1,2-bis[di(sulfonatophenyl)phosphinomethyl]cyclobutane, tris(para-phosphnatophenyl)-phosphine, bis(meta-sulfonatophenyl)(paracarboxyphenyl)phosphine, and bis(metasulfonatophenyl)(2-sulfonatoethyl)phosphine. The Ni catalyst solution is prepared by mixing a degassed aqueous solution of the ligand with Ni(COD)2. The resulting aqueous solution is mixed with previously degassed o-xylene, and the mixture is heated at 45°C for 15 hr before settling into two phases after cooling. The aqueous phase is then combined with an aqueous solution of ZnCl2 and 3-PN before HCN is added to initiate the hydrocyanation.									
US 5488129	Rhone-Poulenc Fiber & Resin Intermediates	11/3/93	3-PN	Ni(COD)2, Sulfonated triphenylphosphine and ZnCl2	60-65	--	2.0	>89	97-99 to ADN, MGN, ESN and VN (yield)
Trisulfonated triphenylphosphine is used for the preparation of the Ni catalyst solution. Initially, the phosphine in aqueous solution is degassed before it is mixed with Ni(COD)2. The resulting aqueous solution is mixed with o-xylene, which is also degassed. The resulting mixture is heated at 45°C for 15 hr before settling into two phases after cooling. The aqueous phase is then combined with an aqueous solution of ZnCl2 and 3-PN before HCN is added to initiate the hydrocyanation. The by-products are methylglutaronitrile (MGN), ethylsuccinonitrile (ESN), and valeronitrile (VN). Linearity, which is defined as ADN/(ADN+MGN+ESN), is 60-89%.									
WO 99/52632	DuPont	4/16/98	Butadiene, 2M3BN, or 3-pentenenitrile	Ni(COD)2 and bidentate phosphorus ligand	--	--	--	--	--
The bidentate phosphorus ligands are prepared first by reacting PCl3 with pyrrole in toluene in the presence of TEA. The resulting slurry is further reacted with 2,2'-biphenol or 1,1'-binaphthol also in the presence of TEA. Indole can replace pyrrole, and other diols, such as 2,2'-3thiylidenebis(4,6-dimethylphenol) and bis(2-hydroxy-1-naphthyl)methane, can also be used in the place of 2,2'-biphenol for the preparation of the bidentate phosphorus ligands. The catalyst systems are used for hydrocyanation of butadiene, isomerization of 2M3BN, or hydrocyanation of 3-pentenenitrile (3-PN). In the latter case, a Lewis acid, such as ZnCl2, is used as a promoter.									

Table 4.5 (Concluded)
TECHNOLOGY FOR HEXAMETHYLENEDIAMINE

PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	Catalyst	Temperature (°C)	Pressure (MPa)	Reaction Time (hours)	Reaction Conversion (%)	Reaction Selectivity (%)
Hydrocyanation of Pentenenitrile (concluded)									
US 5312959	DuPont	7/12/93	--	--	--	--	--	--	--
ADN is produced from butadiene by two-step hydrocyanation in the presence of a Ni catalyst and a boron-compound promoter, such as triphenyl borane or phenyl boronic acid. The reaction mixture contains ADN, 2-methyl glutaronitrile (MGN), phenyl t-butylcatecholboronate (PBCB), triphenyl boron, phenyl boronic acid, and other organic compounds. The PBCB is a reaction product of t-butyl catechol and the boron compound. T-Butyl catechol serves as polymerization inhibitor in the butadiene feedstock. The mixture is distilled in a first column to remove MGN, PBCB, and other volatile organic compound as an overhead. The bottom stream comprising ADN and other boron compounds is mixed with excess ethylene glycol before sending to a second column, where ADN free of boron compounds and t-butyl catechol is recovered. The overhead from the second column is combined with the overhead from the first column. The resulting mixture is further distilled in a series of two more distillation columns to recover MGN.									
Hydrogenation of Adiponitrile									
US 5900511	DuPont	3/26/98	ADN	Cr and Ni modified Raney Co catalyst	75	3.6	10	100	97-99
ADN is continuously hydrogenated to HMDA in an autoclave in the presence of Raney Co catalyst and in a reaction medium substantially free of caustic. Aqueous ammonia is added to the reaction mixture to control the content of bis(hexamethylene)triamine (BHMT), a dimer of HMDA, in the mixture, and to rejuvenate the catalyst.									
US 5726334 US 5599962 US 5559262	DuPont	1/31/95	ADN	Complex of Ru with phosphorus ligand	80-100	7.0	3.4-20.5	100	94-99
ADN is hydrogenated to HMDA in the presence of a Ru complex catalyst with an organophosphine ligand. Preferred catalysts are RuH ₂ (N ₂) ₂ (PCy ₃) ₂ , RuH ₂ (H ₂) ₂ (PCy ₃) ₂ , RuH ₂ (N ₂) ₂ (P-iPr ₃) ₂ , and RuH ₂ (H ₂) ₂ (P-iPr ₃) ₂ , where Cy is cyclohexyl group and iPr is isopropyl group. These complexes are prepared from Ru(COD)Cl ₂ (COD is 1,5-cyclooctadiene) and a phosphine, such as PCy ₃ or P-iPr ₃ , in the presence of NaOH, benzyltriethylammonium chloride (as phase-transfer catalyst) and a solvent selected from benzene and toluene. The longer the reaction time, the higher the ADN conversion and the selectivity to HMDA.									
US 5840989	Rhone-Poulenc Chimie	12/16/94	ADN	Raney nickel doped with Ti or Cr	≤ 100	2.5	2	100	95-97
ADN is hydrogenated to HMDA in a mixed solvent, consisting of HMDA, ethanol and water (60:30:10 by weight) or HMDA and water (98:2 by weight). The reaction takes place in the presence of the doped Ni catalyst and a small amount of alkali metal hydroxide. The by-products are hexamethyleneimine, azacycloheptene, diaminocyclohexane, aminoethylcyclopentylamine, N-ethylhexamethylenediamine, and bishexamethylene triamine.									
US 5801286 US 5777166	Rhone-Poulenc Chimie	12/28/93	ADN	Raney nickel doped with Ti or Cr	80	2.5	2	100	95-97
ADN is hydrogenated to HMDA in a mixed solvent, consisting of HMDA, ethanol and water (63/31.5/5.5 by weight) in the presence of the catalyst and a small amount of caustic soda. The by-products are the same as those described in US 5840989.									
Purification of HMDA									
US 6139693	BASF	2/7/97	--	--	--	--	--	--	--
The reaction mixture from partial hydrogenation of ADN comprises HMDA, hexamethyleneimine, 2-aminomethylcyclopentylamine, 1,2-diaminocyclohexane, ADN, and 6AMCN. It is distilled in a series of three or more columns to recover purified HMDA.									

Table 4.6
TECHNOLOGY FOR NYLON 66
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	MW Regulator	Catalyst	Diluent	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)
US 6103863 US 6084056	DuPont	12/22/98	Adiponitrile (ADN) HMDA	--	A mixture of phosphorous acid and Ca-hypophosphite	Water	270	1.8	3
<p>ADN is hydrolyzed with water in the presence of phosphorous acid and calcium hypophosphite at 200-300°C under nitrogen at 0.5 MPa for about 6 hr. A small amount of ADA is also added as cocatalyst. The resulting hydrolysate is then heated to 270°C and reacts with HMDA for 0.5 hr to produce nylon 66 with a bis(hexamethylene)triamine (BHMT) level of less than 250 ppm.</p>									
US 6075117	DuPont	12/21/98	ADN and HMDA	--	ADA	Water	230 or 250	2.8	4.0
<p>ADN is hydrolyzed with water in the presence of ADA with no additional catalyst. The amount of ADA is about 15-20 wt% based on the amount of ADN. The resulting mixture comprises 15-32 wt% adipamide, 25-35 wt% adipamic acid, 7-10 wt% ADA, and small amounts of 5-cyanovaleramide and 5-cyanovaleric acid. The resulting hydrolysate is then heated to 275°C and reacts with HMDA for 20-45 minutes to produce nylon 66 with a bis(hexamethylene)triamine (BHMT) level of less than 300 ppm.</p>									
US 6011134	DuPont	1/30/98	MADP and HMDA	--	--	--	120-150	--	--
							270-280	--	10-45 min.
<p>Nylon 66 is prepared directly from HMDA and monomethyladipate (MADP) in the presence of water at 10-50 wt% based on the total amount of reactants. Polymerization takes place in two steps. Initially, HMDA and MADP, in an approximately equimolar ratio, are reacted at 120-150°C. Methanol formed during the reaction is removed at an amount at least 90 mol% of the theoretical stoichiometric amount. The resulting aqueous solution is heated to 200-260°C to distill off all the water at 0.7-1.7 MPa. The distillation residue is then subjected to final polycondensation at 270-280°C and atmospheric or sub-atmospheric pressure for 10-45 min to produce nylon 66 with less than 50 mols of N-methylhexamethylenediamine per million grams of the polyamide. The presence of N-methylhexamethylenediamine at greater than 50 mols per million gram results in poor polymer quality.</p>									
US 5801278	DuPont	3/7/97	ADA and HMDA	--	--	--	--	--	--
<p>ADA reacts with HMDA in the presence of water at 2-5 wt% based on the weight of reaction mixture. Initially, ADA powder is mixed with dry ice at an ADA:dry ice weight ratio of 1:0.5-1:1 in a mixer. An aqueous solution containing 91.3 wt% HMDA heated to 45°C is then added to the mixer over a period of 15 min. The resulting mixture is blended for 1 hr. The resulting reaction mixture is in substantially solid particulate form.</p>									
US 5955569	DuPont	11/27/96	Nylon 66 salt	--	--	--	175-200	--	--
							250-275	--	--
<p>Polyamide moist pellets, having low relative viscosity, are treated with a low dew point (<30°C) nitrogen gas in a solid-phase polymerization vessel. The use of low dew point nitrogen provides a driving force for diffusion of moisture from the interior to the surfaces of the polyamide pellets and evaporation of the water from the surfaces. The polyamide pellets, containing 2(2'pyridyl)ethyl phosphonic acid, is prepared by first mixing an aqueous nylon 66 salt solution with the phosphonic acid catalyst. The mixture is heated to remove excess water. Upon reaching to 10-30 wt% water, the reaction mixture is transferred to an autoclave for a second stage polymerization, where the reaction temperature is increased first to 175-200° and then to 250-275°C. The resulting polymer is then extruded into pellets, which is subjected to the solid-phase polymerization to increase MW to a desired level.</p>									
US 5731403	DuPont	7/30/96	ADA and HMDA	--	--	--	< 180	--	--
<p>Nylon 66 is prepared by reacting an ADA-rich mixture, containing 71-81 wt% ADA and 29-19 wt% HMDA, with anhydrous HMDA at a temperature lower than 180°C so that substantial evaporation of HMDA during the reaction is avoided.</p>									

Table 4.6 (Continued)
TECHNOLOGY FOR NYLON 66
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	MW Regulator	Catalyst	Diluent	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)
US 5824763	DuPont	8/25/95	Nylon 66 salt and ADA	Acetic acid	Sodium hypophosphite	--	235 283	1.55 to 0.1 <0.1	?
A nylon 66 salt solution (51.5 wt%) is preheated to 55°C and mixed with ADA and acetic acid solutions. The resulting mixture is prepolymerized at 235°C and 1.55 MPa to produce low MW polymer, which is discharged to a flasher. The pressure in the flasher is reduced to further remove water vapor. The polymer is finally discharged to a vent extruder at 283°C and under vacuum. The resulting polymer is extruded and pelletized. The nylon resin has an acid/amine end group ratio of greater than 4:1, depending the amount ADA added, and has a high melt flow of 30-49 g/10 min at 280°C.									
US 5665854	DuPont	3/24/95	--	--	--	--	--	--	1.0
Free flowing nylon 66 particles are produced from HMDA and CO ₂ in two step polymerization at reaction temperatures below the melting point of the initial materials. Prepolymerization takes place at 160°C for >10 hr in the first step, and solid-phase polymerization takes place at 230°C for 6-18 hr in the presence of small amounts of 6-aminohexanoic acid to produce nylon 66 with high relative viscosity of 100-138.									
US 5674974	DuPont	11/23/94	Acid-rich molten mixture and HMDA	--	--	--	120-135	--	1-3
Nylon 66 is prepared continuously in a vertical multiple-stage reactor with internals, such as perforated plates, coils, and agitators, which provide effective contact of countercurrently flowing diamine stream with a molten acid-rich stream. Initially, the molten acid-rich mixture is continuously prepared in an agitated reactor, into which solid granular ADA and liquid HMDA or >85 wt% HMDA aqueous solution are added at 120-135°C for 1-3 hr holding time. The resulting molten acid-rich mixture, containing 81 wt% ADA and 19 wt% HMDA is withdrawn and fed into the top of the vertical 8-stage reactor with HMDA countercurrently fed into the reactor at various stages 2 through 8. A near infrared analysis system (UOP/Guided Wave Model 300P near-infrared spectrometer) is used to control the desired ADA/HMDA ratio in the molten mixture by injection of necessary amount of HMDA into the reactor. The resulting polymer has a number average MW of 10500-11000. The loss of diamine through the polymerization reactor is less than 100 ppm based on the polymer.									
US 6107449	Polymer Engineering GmbH	5/24/96	HMDA and ADA	--	--	--	--	--	--
ADA/HMDA salt (AH salt) at 60-80 wt% aqueous solution is heated to 90-100°C in a first holding vessel. The solution is further heated and sent to a second pressure reactor, where polymerization proceeds under 26 bar without removal of volatiles. The resulting low-viscosity polymer is then heated to 280°C to evaporate the excess water in a third reactor, which is equipped with a rectification column and an immersion vessel under a pressure of 3 bar. The resulting prepolymer is transferred to a post condensation reactor, where hot nitrogen is used to purge more water from the reaction mixture. The resulting nylon 66 has a solution viscosity of 2.6. For nylon 66 with a solution viscosity of 3.3, two additional post condensation reactors are necessary.									
US 6136947	Polymer Engineering GmbH	12/12/95	--	--	--	--	--	--	--
Nylon 66 or copolyamide of nylon66 and nylon6 is polymerized in a similar process as described in US 6107449.									
US 5686556	Rhone Poulenc Chimie	1/25/93	HMDA and dimethyl adipate	--	Na-methylete	--	50 200-270 270	-- -- --	2-5 1.0 5.0
Nylon 66 is prepared from α -amino ω -ester monoamide, which in turn is prepared from HMDA and dimethyl adipate. In the process, HMDA is melted in a reactor, into which dimethyl adipate is added; the resulting mixture reacts at 50°C under nitrogen in the presence of a catalyst active for aminolysis reaction, such as sodium methylate, alkali metal aryloxides and organic titanium or zirconium compounds. The molar ratio of diamine to diester is between 1:1 and 1.1:1. At such a low temperature of reaction, the ester monoamide precipitates as soon as it is formed. The resulting solid is washed with water to remove unreacted compounds. The ester monoamide is then heated at reflux for 1 hr at a temperature varying from 200°C to 270°C to carry out oligomerization with methanol vigorously released from the reaction mixture. The reaction continues at 270°C for additional 5 hr.									

Table 4.6 (Concluded)
TECHNOLOGY FOR NYLON 66
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown	Major Reactants	MW Regulator	Catalyst	Diluent	Reaction Temperature (°C)	Reaction Pressure (MPa)	Reaction Time (hours)
US 6169162	Solutia	5/24/99	ADA and HMDA	--	--	--	260	1.1	--
260-280 atmospheric --									
Solid ADA is subjected to a vacuum and inert gas purge to reduce oxygen content before it is melted in a vessel made of Hastelloy C or stainless steel 316, and mixed with molten HMDA in equimolar amounts through an in-line mixer. The resulting mixture is sent to a first reactor at 260°C and 1.1 MPa to produce a partially polymerized nylon 66 reaction mixture. Water formed during the polymerization is removed through a HMDA recovery column. The prepolymer from the first reactor passes to a second vertical reactor, where the mixture is further polymerized at 260-280°C and atmospheric pressure. The resulting polymer is pelletized and dried before it passes to product storage.									
US 5627257	Zimmer Ag	5/27/94	ADN and HMDA	--	A mixture of phosphorous acid and Ca-hypophosphate	Water	230 270	2.5 1.0	5.0 0.5-1.0
ADN is hydrolyzed with water in the presence of phosphorous acid and calcium hypophosphate at 230°C under nitrogen at 2.5 MPa for about 5 hr. ADA is also added at 15 wt% of ADN as cocatalyst. Reportedly up to 95% of ADN is converted to ADA. The resulting hydrolysate is then heated to 270°C and reacts with HMDA for 0.5-1.0 hr to produce nylon 66 with a bis(hexamethylene)triamine (BHMT) level of less than 600 ppm.									
Solid-Phase Polycondensation									
US 5140098	BASF	9/29/89	Polyamide	ADA and HMDA	--	--	180-190	--	8
Linear high MW polyamides, such as nylon 66 are prepared by solid-phase polycondensation of polyamide from a previous stage polymerization with ADA (at 0.25 wt% based on the polyamide). The polyamide and ADA are mixed, extruded and cut into granules, which is subjected to solid-phase polycondensation to produce high MW polyamide. The resulting polyamide is suitable for the manufacture of fibers and filaments. It also can be formed into shaped articles by extrusion or injection molding. In the latter case, reinforcing agents, such as glass fibers or silicate fillers are added to the extruder, where the polyamide and ADA are mixed.									
US 5874520	DuPont	9/15/97	6-Aminohexylcarbamic acid and ADA	--	--	--	?	--	5 min
6-Aminohexylcarbamic acid [NH ₂ (CH ₂) ₆ NHCOOH] and ADA is ground/mixed in a single bladed laboratory mixer for 5 min to produce nylon 66 salt.									

Table 4.7
TECHNOLOGY FOR NYLON RECLAIM
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown
US 5929234 US 5932724 US 5681952	AlliedSignal/DSM N.V.	5/21/98 4/16/97 12/8/95
A shredded nylon 6 carpet, containing nylon 6 face fiber (52-58 wt% nylon 6), polypropylene backing, and calcium-filled SBR, is extruded and further ground into 5 mesh chips. The chips are subjected to depolymerization in a cylindrical stainless steel reactor at 300-340°C with superheated steam. After a total 5-6 hrs of depolymerization, decomposed products are condensed to a yield of CAPM of 89.9% based on nylon 6 in the carpet scraps.		
US 5722603	AlliedSignal/DSM N.V.	11/28/95
A waste carpet, containing nylon 6 face fiber, polypropylene backing, and SBR latex adhesive compounds is initially subjected to size reduction by shredding or cutting in a rotor shredding machine. This operation is to separate adhesive material by dry screen separation. If necessary, a second size reduction by a hammer mill can be used to remove additional residue adhesive material. The dry separation provides a mixture, which contains about greater than 90 wt% of face fiber based on the waste carpet feed stock. The mixture is then washed with water in three stages. Some additives, such as surfactant and caustic soda can be added during the washing to enhance the removal of oils, dyes, soil repellents, and stabilizers in the face fiber, and to reduce the bonding strength between the face fiber and backing mixture as well as compounded latex. After washing, the mixture is subjected to a fluidic separation through a series of three hydrocyclones to separate the face fiber from the backing materials.		
US 5990306	AlliedSignal	9/3/97
A waste carpet, containing nylon 6 face fiber, is depolymerized in the presence of steam at 300-340°C and 1.5 MPa to obtain a mixture of crude CAPM and water. The reaction mixture is filtered through a filter aid, such as diatomaceous earth to remove an emulsified layer, and treated with caustic soda if the waste carpet contains PET fiber. The resulting mixture is concentrated or distilled to remove most of water, and flashed at 110-150°C and 2-6 mmHg. The CAPM from the flasher is dissolved in small amount of water (2-12 wt%) at < 65°C, and the resulting solution is crystallized to obtain CAPM, which is recovered by filtration and washed with pure CAPM or lactam solution.		
US 5889142	AlliedSignal	4/21/97
A mixture of CAPM and water containing 40 to 50 wt percent of the latter is used to dissolve nylon from nylon waste materials at 150-160°C for 30 minutes, and to separate the remaining mass, such as carpet backing. The polymer is recovered without degradation under normal manufacturing conditions.		
US 5948908 US 5869654	AlliedSignal	3/18/96 3/18/96
A shredded nylon 6 carpet, containing nylon 6 face fiber (52-58 wt% nylon 6), polypropylene backing, and calcium-filled SBR, is extruded and further ground into 5 mesh chips. The chips are subjected to depolymerization in a cylindrical stainless steel reactor at 300-340°C with superheated steam. After a total 5-6 hrs of depolymerization, decomposed products are condensed to a yield of CAPM of 89.9% based on nylon 6 in the carpet scraps.		
US 5656757	AlliedSignal	8/10/95
Carpet wastes strips are shredded and melted in an extruder. The melted nylon wastes are subjected to hydrolytic depolymerization with water at 295°C in a series of three reactors. The resulting mixture is cooled to 70-95°C to separate water insoluble components. The water soluble depolymerization products are concentrated and distilled to get purified CAPM. Water from concentration and distillation is recycled to the hydrolytic depolymerization reactor.		
US 5457197	AlliedSignal	4/8/94
Shredded carpet wastes are extracted with water at 290°C for 10-30 min. A superheated steam is then sparged through the aqueous mixture at 330°C for more than 3 hr to hydrolytically depolymerized the nylon waste.		

Table 4.7 (Continued)
TECHNOLOGY FOR NYLON RECLAIM
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown
US 4311642	Allied Corp.	9/17/80
	The wash water from nylon 6 production contains water, CAPM and cyclic oligomer. It is subjected to evaporation in a wiped-film evaporator under 200-300°C and 10-250 mmHg to separate an overhead stream of water and CAPM, and a bottom stream of CAPM and cyclic oligomers. The overhead stream is distilled to recover CAPM, and the cyclic oligomers in the bottom stream are 85% depolymerized at 230-290°C to recover CAPM, which is stripped by superheated steam.	
US 5495015	BASF	12/12/95
	CAPM is recovered from nylon 6 wastes in the presence of superheated water at 250-320°C and 7.5-15 MPa for about 1 hr. The weight ratio of water to polymer ranges from 5:1 to 13:1. The yield of CAPM is about 90-96%.	
US 5700358	BASF	3/4/94
	Crude CAPM from depolymerization of nylon 6 wastes is dewatered by distillation. It is then distilled with 0.3 wt% sulfuric acid in a column packed with Raschig rings under 0.5 kPa. The distillate is further distilled with 0.25 wt% caustic soda in a second column packed with Sulzer packings under 0.5 kPa and a bottom temperature of 130°C.	
US 5294707	BASF	2/25/93
	Nylon 6 is semi-continuously depolymerized with superheated steam in the presence of phosphoric acid as a catalyst. The depolymerization is carried out to a relatively low degree of conversion before recharging the depolymerization reactor with a new batch of nylon 6 waste. For catalysts which are polymerizable, such as ortho-phosphoric acid and p-toluenesulfonic acid, the degree of conversion prior to recharge of nylon waste is preferably 40 to 85 %, while for non-polymerizable catalysts, such as boric acid and 4-sulfoisophthalic acid, the degree of conversion is 75 to 90 %. The reactor is purged with nitrogen or some other inert gases during the addition of polymer waste because of the sensitivity of catalysts to oxygen. The catalyst is added as an aqueous solution with preferred concentration in the range of from 40 to 85 wt% in a one-time load in the process for a total of 50 charges. The reaction temperature is between 260° and 280°C.	
US 5977193	BASF	9/11/92
	CAPM is continuously recovered from carpet wastes. In the process, the carpet waste in strips is fed into a separator, where the strips are shredded and a large portion of non-CAPM materials, such as latex, jute and polypropylene, are mechanically removed. The nylon 6 waste from the separator is fed to a depolymerization reactor along with nylon wastes from other sources. The reactor can be operated continuously, batchwise, or semi-continuously. Depolymerization is carried out at 250° to 280°C with superheated steam in the presence of phosphoric acid. From the depolymerization reactor, a distillate, containing CAPM, water and other non-aqueous volatiles is fed to a fractionating column to recover crude CAPM, which is subjected to oxidation treatment at 40-50°C with KMnO4 before being further concentrated and distilled to obtain pure CAPM.	
US 6140428	BASF	6/17/92
	Nylon 66 waste is comminuted to 8 mm particles, which are mixed with 15 wt% caustic soda in methanol. The resulting mixture is heated to 180°C for 4 hr, and cooled to precipitate sodium adipate. The solids are filtered and washed repeatedly with methanol and dried. The dried sodium adipate is further purified by forming an aqueous solution, which is treated with activated carbon and with selective ion exchange resin. The mother filtrate is combined with filtrates from the methanol washes; the resulting mixture is distilled first to recover methanol at atmospheric pressure. The distillation residue is further distilled to recover HMDA.	
US 5359062	BASF	5/7/92
	Nylon 6 wastes are hydrolytic depolymerized with 5-30 parts by weight of water per part of nylon 6 at 200°-350°C and a pH of 5-10 in the presence of sodium hydroxide.	
US 6020486	DSM N.V.	7/14/97
	Nylon 6 waste is depolymerized at 270°C for 1-4 hr in ethylene glycol in the presence of phosphoric acid, phosphorous acid, polyphosphoric acid, or alkali metal salts of methanol or ethanol. The conversion is about 27-32.5 %.	

Table 4.7 (Continued)
TECHNOLOGY FOR NYLON RECLAIM
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown
US 6087494	DSM N.V.	5/1/97
	Nylon 6 waste is depolymerized at 270°C for >3 hr in the presence of small amounts of caustic soda (0.15 wt% based on the polyamide to be depolymerized). The depolymerization is carried out by passing steam through the molten polyamide at the rate of 3.5 kg per kg of polyamide feed. The steam leaving the depolymerization reactor is cooled and condensed. The monomer is recovered by vacuum distillation.	
US 6111099	DSM N.V.	7/12/95
	Nylon 6 carpet is shredded in pieces, and mixed with water, which is recycled from the extraction at later stage of operation. The resulting heterogeneous mixture is subjected to depolymerization at 300°C and 10.0 MPa for 1 hr. After the reaction, the mixture is cooled and depressurized to remove part of water, and filtered to remove solid particles. The filtered mixture is extracted with dodecyl phenol to recover virtually all CAPM, cyclic oligomers and some water. The resulting organic mixture is distilled to recover a mixture of CAPM and water, which is further treated with ion exchanger and then hydrogenation. After the treatment, CAPM is recovered by distillation at 116°C and 5 mbar.	
US 5556890	DSM N.V.	6/4/93
	Industrial carpet waste, containing nylon 6 face fiber, latex adhesive, polypropylene backing and calcium carbonate filler, is shredded and mechanically separated to obtain a mixture of nylon 6 and non-nylon 6 carpet waste (95 wt% nylon 6). The mixture is subjected to depolymerization at 280-290°C for 2 hr with superheated steam in the presence of phosphoric acid. After the reaction, the distillate from the depolymerization reactor is concentrated to an aqueous solution of 30 wt% CAPM, which is hydrogenated at 90°C and 0.5 MPa for 1 hr. The resulting mixture is decanted to remove most of the catalyst followed by filtration to remove the residual catalyst. After neutralized with small amount of caustic soda, the filtrate is distilled to recover CAPM.	
US 5750791	DuPont	8/20/96
	Nylon 66 waste is subjected to hydrolysis at 103-106°C with nitric acid while avoiding significant oxidation of diamine to diacids, such as adipic acid, glutaric acid and succinic acid. In the process, the nylon waste is washed to remove dirt, dyes, etc., and are fed to hydrolysis reactor, where it is mixed with a nitric acid solution at 18-35 wt%. The mixture is heated at reflux. After 6 hr, the hydrolysis solution is filtered to remove sludge containing carpet backing components and other solids before it is cooled to crystallize ADA, which is recovered by filtration and rinsed with cold water. The filtrate is hydrogenated to convert nitric acid to ammonia in the presence of a hydrogenation catalyst, such as Pt, Pd or Ni. The reaction mixture is filtered, and stripped to remove ammonia and some water. The stripped liquid is distilled to recover HMDA.	
US 5468900	DuPont	9/29/94
	Wastes of nylon 6 and/or nylon 66 are depolymerized in the presence of an aliphatic acid, such as acetic acid or propionic acid and the depolymerized products are further converted to ADA by oxidation. In case of nylon 6 waste, at least one mole of the aliphatic acid is used for every mole of repeat unit of the polymer during the depolymerization. In case of nylon 66 waste, at least two moles of the aliphatic acid are used for every mole of repeat unit of the polymer. The depolymerization products are 6-acetoamidohexanoic acid in the nylon 6 case, and ADA and N,N'-hexamethylene bisalkylamide in the nylon 66 case. These depolymerization products are oxidized either chemically or electrochemically to ADA. For chemical oxidation, the catalyst is composed of cobaltous acetate, manganese acetate, and 48 wt% HBr solution. The oxidation is carried out in the presence of acetic acid at a temperature between 93° and 104°C for 24 hr. The conversion is about 50-60% with a yield of ADA at less than 25% on a molar basis. For electrochemical oxidation, the reaction is carried out in an electrolytic cell with a cell voltage of about 3 volts and parallel platinum electrodes in the presence of cobaltous acetate and sulfuric acid solution. The conversion is also about 50-60% with a yield of ADA at 70% from 6-acetoamidohexanoic acid on a molar basis, and less than 20% from N,N'-hexamethylene bisacetamide on a molar basis.	
US 5310905	DuPont	4/14/93
	Waste of nylon 6 and/or nylon 66 is depolymerized in the presence of acetic acid to a mixture of CAPM, ADA, 6-acetamidohexanoic acid, and N,N'-methylene bisacetamide.	
US 5266694	DuPont	10/19/92
	Waste of nylon 6 and/or nylon 66 is depolymerized by steam distillation in the presence of caustic soda to obtain CAPM and ADA with low yields.	

Table 4.7 (Continued)
TECHNOLOGY FOR NYLON RECLAIM
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown
EP 603434	Karl Fischer Ind.	6/29/94
Nylon 6 is recovered from Nylon waste, which contains 80 wt% nylon 6 and 20 wt% polypropylene. The waste material is dissolved in 85 wt% formic acid at 40°C for 30 min. After removing the indissoluble polypropylene, the nylon 6 the remaining solution is precipitated with a dilute formic acid. It is recovered, washed and dried.		
JK 11021347	Nippon Polypenco	7/1/97
Fifty grams of nylon 6 scraps are completely depolymerized in the presence of 500 ml of molten CAPM at 150°C for 24 hr. The operation is repeated for 10 times to obtain a mixture of 500 ml CAPM and 500 ml of depolymerized product. The mixture is subjected to anionic polymerization in the presence of small amounts of NaH and TDI to regenerate nylon 6.		
US 5646191	Polymer Engineering	1/28/93
Nylon waste is melted in an extruder, and filtered to remove impurities not consisting of nylon 6. The melt undergoes hydrolysis in a pressure reactor, which is equipped with a device made from expanded metal or perforated plate. The device is to increase active surfaces for the melt to flow downward in thin layers. Water is heated and added along with the melt in a controlled amount, which is effected as a function of the pressure in the reactor. One portion of the affluent from the hydrolysis reactor passes through a shearing filter before it is recycled back to the hydrolysis reactor. The shearing filter serves the purpose of linearly deforming the spherical particle gels into stretched polymeric molecules, which is more easily hydrolyzable. A second portion of the affluent passes to a second reactor, which is also equipped with a similar device as that in the first reactor. The second reactor is either under vacuum or nitrogen purge to recover CAPM and steam from the top of the reactor. The bottom stream from the second reactor is recycled to the first one. A third and lastly portion from the first reactor is transferred to nylon polymerization.		
US 6036726	Solutia	10/27/95
A process for removal of colorant from nylon 66 waste is cited. The colored nylon waste is dissolved in an alcohol along with water at 160-180°C. Nylon is separated from the other components in the nylon waste by precipitation from the solution.		
JK 6032775	Sumitomo	5/18/92
Nylon 6 waste is depolymerized at 150-160°C in the presence of phosphoric acid and a Lewis acid, such as p-toluene sulfonic acid or trifluoromethane sulfonic acid. Addition of Lewis acid improves the yield of CAPM.		
JK 11240979	Toray	2/25/98
Nylon 6 waste pulverized in a cutter mill is depolymerized at 260°C with steam in the presence of 75 wt% phosphoric acid for 3 hr. The resulting distillate contains 10.4 wt% CAPM with 92% CAPM recovery. The solution is concentrated to 95 wt% CAPM with 0.97 wt% impurities under 55°C and 30 mmHg. The concentrate is further distilled under 150-170°C and 5 mmHg with 95% recovery of CAPM having 0.5 wt% impurities.		
JK 8217746	Toray	2/9/95
Nylon 6 waste, containing 90 wt% nylon 6, is depolymerized at 260°C with steam in the presence of 75 wt% phosphoric acid for 6 hr. The resulting distillate contains 7.7-9.9 wt% CAPM with 94% CAPM recovery. The solution is concentrated to 95 wt% CAPM with about 1 wt% impurities under 55°C and 30 mmHg. The concentrate is added with a small amount of 20 wt% caustic soda solution, and the resulting mixture is further distilled under 165-180°C and 5 mmHg with 81-84% recovery of CAPM having < 0.1 wt% impurities.		
JK 7330718 JK 7330717 JK 7330716	Toray	6/9/94
Pulverized nylon 6 waste is melted at 300°C. The resulting melt passes through a metal trap to remove metallic impurities. The melt overflows the metal trap to a reactor, where it is subjected to depolymerization with steam in the presence of 75 wt% phosphoric acid.		

Table 4.7 (Concluded)
TECHNOLOGY FOR NYLON RECLAIM
PATENT SUMMARY

Reference Number (Patent)	Assignee	Earliest Date Shown
JK 8048666	Toray	6/1/94
Nylon 6 waste, containing 90 wt% nylon6, is depolymerized at 260°C with steam in the presence of 75 wt% phosphoric acid for 7-10 hr. The resulting distillate contains 6-9 wt% CAPM with 80-90% CAPM recovery. The solution is concentrated to 96 wt% CAPM with 2.1 wt% impurities under 55°C and 30 mmHg. The concentrate is dissolved in trichloroethylene, and crystallized to obtain CAPM, which is filtered and rinsed with the solvent. Crystallization provides with 75-80 % recovery of CAPM, which has < 0.05 wt% impurities.		
JK 726013 JK 726014	Toyobo	7/8/93 7/6/93
The extraction water from Nylon 6 production is treated with 20 wt% caustic solution followed by distillation to get crude CAPM containing 67 wt% oligomer. This crude CAPM is combined with nylon 6 waste from spinning operation and crude CAPM from depolymerization of nylon scraps. The resulting mixture is depolymerized with superheated steam at 320°C in the presence of ortho-phosphoric acid to recover CAPM with 92 % yield.		
JK 11035554	Unitika Ltd.	7/15/97
Extract water from nylon 6 production is distilled to recover CAPM; the residue is combined with nylon 6 waste. The resulting mixture is subjected to depolymerization at 280°C for 6 hr with superheated steam in the presence of phosphoric acid. The resulting aqueous CAPM solution is mixed with 30 wt% caustic soda to adjust its pH to 12.5 before it is subjected to a treatment with activate charcoal. The treated water solution is distilled to recover CAPM with high purity (1.5-2.5 ppm adipimide).		
JK 10298162	Unitika Ltd.	4/25/97
Nylon 6 waste is depolymerized at 300°C by steam in the presence of 80 wt% phosphoric acid for 5 hr. The distillate from the depolymerization reactor contains a mixture of CAPM, water and small amount of valerolactam. It is concentrated from about 15.8 wt% CAPM to 95 wt% at 60°C under 30 mmHg. The resulting solution is further distilled under 110-120°C and 1 mmHg to obtain CAPM with 35 ppm valerolactam. Alternatively, extract water from nylon 6 production can be combined with the distillate from depolymerization of nylon 6 waste. The resulting mixture is then concentrated to 95 wt% CAPM under 60°C and 30 mmHg, and the resulting mixture is dissolved in n-hexane. The solution is filtered before it is cooled to crystallize CAPM, which contains 20 ppm valerolactam.		
JK 10287645	Unitika Ltd.	4/11/97
Extract water from nylon 6 production is distilled to recover CAPM, the residue is combined with nylon 6 waste. The resulting mixture is subjected to depolymerization at 280°C for 6 hr with superheated steam in the presence of phosphoric acid. The resulting aqueous CAPM solution is concentrated to 95 wt% under 60°C and 30 mmHg. The concentrated solution, containing 45 ppm adipimide, is further distilled under 110-130°C and 1 mmHg to recover CAPM 1.5 ppm adipimide. Alternatively, the concentrated solution is mixed with n-hexane and heated to dissolve CAPM. After filtration to remove solids, CAPM is slowly cooled to crystallize. The CAPM is recovered and dried to have the adipimide content of <0.1 ppm.		
DE 4316408	Zimmer	5/17/93
Nylon6 carpet waste is depolymerized with steam in the presence of phosphoric acid. The distillate is concentrated to 50 wt% solution followed by adding KMnO4 crystals at 40-60°C for about 15 min. The amount of free permanganate in the solution, at no time, exceeds 0.4 wt% with respect to CAPM. The solution is then treated with active carbon and filtered. The filtrate is vacuum distilled to give high-purity CAPM.		

Appendix B

DESIGN AND COST BASES

DESIGN AND COST BASES

DESIGN CONDITIONS

Design and cost calculations are based on an assumed plant location along the U.S. Gulf Coast at Houston, Texas. Particular temperature assumptions are:

Dry bulb air temperature	38°C (100°F)
Wet bulb air temperature	27°C (80°F)
Groundwater temperature	27°C (80°F)
Cooling water temperature	29°C (85°F)
Cooling water range	11°C (20°F)

The usual definitions of terms relating to yield are used in this report. They are as follows:

- | | |
|----------------|--|
| Conversion | Ratio of material reacted to material fed, stated in percent or fraction |
| Selectivity | Ratio of product desired to material reacted, stated in percent or fraction of material reacted |
| Yield per pass | Ratio of product desired to material fed, stated in percent or fraction of material fed = Conversion x Selectivity |

COST BASES

Below, we outline the criteria for calculating capital investment and production costs, and the effect of the operating level on production costs.

Capital Investment

Equipment costs are estimated primarily from correlations developed by PEP and supplemented occasionally by vendors' estimates. If an equipment item is specialized or contributes substantially to the cost of the facility, a vendors' quote has been obtained if possible. When necessary, the costs are corrected to a PEP Cost Index of 624.

Direct installation costs are estimated by a modular method developed by PEP; the details are described in PEP Report 145, *Battery Limits Cost Estimating* (April 1982). The indirect costs in capital investment are estimated by adding allowances for engineering, field expenses, overhead, purchasing, and contractor's profit. The bases for the estimation of these allowances are detailed in Section 7 of PEP Report 162, *Computer Program for Estimating Plant Investment* (March 1985). These indirect cost estimates are then added to the direct investment (fob costs plus direct installation costs) to get the overall installed costs.

Investment in utilities is computed for the entire plant and allocated to each major operation according to use. Indirect costs for utilities and off-site tankage (generally raw material and product storage) are assumed to be 20% of the direct utilities investment.

General service facilities not directly associated with process operations are assumed to be 20% of the battery limits installed cost and utilities-plus-storage investment. An allowance for waste treatment facilities is also made. These allowances are determined prior to the addition of contingencies to the installed costs.

The total fixed capital for the facility includes total investment in battery limits, utilities and tankage, general service facilities, and a contingency. Usually the contingency is taken as 25% each of the battery limits investment and the off-site investment. All of the above investment estimates have been calculated with the aid of SRI's PEPCOST II computer program.

In comparing SRI's estimates with actual plant costs or contractors' estimates, the following should be borne in mind:

- The processes may be the same generally but differ enough in detail to affect costs significantly.
- The estimates may not be strictly comparable because of omission of process sections (for example, by-product recovery) in one or another of the designs.
- Actual plants are frequently overdesigned for reasons unique to the particular situations.
- During periods of rapid escalation of equipment costs, and when long delivery times are anticipated, cost indexes probably are not an accurate reflection of actual costs.
- During periods of depression in chemical plant construction, equipment vendors and engineering contractors will provide goods and services at little or no profit.

Production Costs

The operating labor wages are based on estimated prevailing rates in Houston, Texas. The base rate is derived from U.S. national average rates in industrial chemical plants, corrected to the Houston area on a relative basis for production workers. With an allowance for fringe benefits and a 10% shift overlap assumed, the effective total rate is \$33.58 per hour. The operating labor requirements have been estimated subjectively on the basis of the number of major equipment items in the process. The number of men per shift includes the working foremen. The cost of staff supervision—such as the assistant operating department manager, etc.—is assumed to be included in our allowance for plant overhead.

The total maintenance costs are estimated to be 6% of the battery limits investment. In each case, we have assumed a 50-56 split between materials and labor.

Plant overhead has arbitrarily been assumed at 80% of total labor. It includes all staff personnel located at the plant site, and services directly associated with plant operations and maintenance.

G&A, sales, and research costs are assumed for each product by making allowances for the stage of process development in estimating research expense, and for the character of marketing channels and technical service requirements in estimating selling expense. These estimates are customarily assigned a percentage of the sales value of the product, generally in the range of 5-30%. When actual prices are unknown, we base the G&A, sales, and research expense on the calculated product value (total production cost plus 25%/yr pretax return on fixed capital).

The cost of taxes and insurance is calculated at 2% of total fixed capital. Depreciation is based on 10%/yr of fixed capital.

Effect of Operating Level on Production Costs

Variations in production costs with plant capacity and with operating rate are based on the following assumptions:

- The annual costs of process plant operating labor, control laboratory labor, and operating materials are invariant with plant capacity. Also, the entire process plant labor force remains on the payroll when the plant is operating at reduced capacity or is shut down.

- Investment-related items, including maintenance labor, maintenance materials, taxes, and depreciation, are directly proportional to investment, and their annual cost remains constant with reduced operating rate.
- Corporate overhead charges are constant to various plant capacities, and the annual allocation is also constant, regardless of plant operating rate.
- Production costs generally do not include any allowance for packaging or shipping; i.e., they represent bulk costs, fob plant.
- Working capital is not included in the fixed capital cost, nor are start-up costs. Interest on working capital is not included in the production cost or in the product value.
- Royalties are not included in any of the estimates. Royalties for any given licensed process may vary considerably, depending on terms of the agreement, geographic location, etc. Initial payments or paid-up royalties may be substantial, and they should be considered in specific estimates.
- Annual costs for raw materials and utilities are directly proportional to the annual plant production.

In accordance with the last assumption, unit costs for raw materials and utility consumptions do not change with either plant capacity or operating rate.

Appendix C

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Appendix D

PATENT REFERENCES BY COMPANY

Patent Assignees

Assignee	Patent Number	Chapter(s)
Allied Chem	US 4311642	A
AlliedSignal	US 5457197	4, A
	US 5656757	4, A
	US 5889142	A
	US 5869654	4, A
	US 5948908	4, A
	US 5990306	4, A
Allied Signal and DSM N.V.	US 5681952	4, A
	US 5929234	4, A
	US 5932724	4, A
	US 5722603	4, A
Arco Chemical Technology, L.P.	US 5451701	4, A
	US 5599987	4, A
Asahi Kasei Kogyo Kabushiki Kaisha	US 5973218	4, A
BASF	EP 167975	4, A
	US 4816557	4, A
	US 4879120	A
	US 5441607	A
	WO 9926996	4, A
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	WO 9964155	4, A
	US 5264571	4, A
	US 5495014	4, A
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	US 5495016	4, A
	US 5496941	4, A
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	US 5508465	A
	US 5589600	4, A

Assignee	Patent Number	Chapter(s)
BASF (continued)	US 5684201	A
	US 5693793	4, A
	US 5700358	A
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	US 5756808	4, A
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	US 5874607	4, A
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	US 6030505	A
	US 6048997	4, A
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	US 6140428	A
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	US 6207851	A
	US 6222059	A
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Bayer	CA 2285828	4, A

Assignee	Patent Number	Chapter(s)
Bayer (continued)	DE 4324616	A
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Daicel Chem Ind and Iwai Y	JK 09077705	A
Degussa-Huls	US 5741904	4, A
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DSM N.V.	US 5539106	4, A
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Assignee	Patent Number	Chapter(s)
DSM N.W. and Du Pont (continued)	US 5495041	4, A
Du Pont	EP 336314	A
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	US 5310905	A
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	US 5440067	4, A
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	US 5512695	A
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	US 5693843	4, A
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	US 5981772	4, A
	US 6075117	4, A
	US 6084056	4, A
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	US 5847191	4, A
	US 6020516	4, A
	US 6127567	4, A
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	US 5250726	A
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	US 5359137	A
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	US 5559262	4, A

Assignee	Patent Number	Chapter(s)
Du Pont (continued)	US 5599962	4, A
	US 5665854	A
	US 5674974	4, A
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	US 5723641	4, A
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	US 6069228	4, A
	US 6120700	4, A
	US 6160183	A
	US 6171996	4, A
	US 6171997	4, A
	US 6284927	4, A
	US 6103863	A
	US 5955569	4, A
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Du Pont and DSM N. V.	US 5618983	A
	US 5962732	4, A
	US 6133477	4, A

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Ems-inventa	US 5747634	A
	US 5760164	4, A
Enichem Anic S.r.l.	US 5312987	4, A
	US 5227525	4, A
Fischer Ind GMBH Karl	EP 603434	A
Fuchs H and Basf	US 5359062	A
Grande Paroisse SA	US 5582810	4, A
Idemitsu Petrochem Co	JK 63081129	A
	JK 63081130	A
Kotek R and Basf	US 5294707	4, A
Lurgi Zimmer	US 6093788	4, A
Mitsubishi Chemical Corporation	US 5569803	4, A
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	US 5865958	4, A
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Mitsubishi Kasei	JK 05331281	A
Nippon Polypenco	JK 11021347	A
Polymer Engineering GmbH	US 5962538	4, A
	US 5973105	4, A
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	US 6107449	A
	US 6136947	A
R.P. Fiber & Resin Intermediates	US 5723603	A
	US 5763655	4, A
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Rhodia Fiber and Resin Intermediates	US 6100396	4, A
	US 6147256	A
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	WO 00/37431	A

Assignee	Patent Number	Chapter(s)
Rhodia Fiber and Resin Intermediates (continued)	US 5908805	A
Rhone-Poulenc	US 5686556	4, A
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	US 5227522	4, A
	US 5227523	4
	US 5268505	A
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	US 5488129	4, A
	US 5625096	4, A
	US 5777166	4, A
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	US 5981790	A
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Solutia	US 6036726	A
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Sumitomo Chemical Company, Limited	US 5502184	4, A
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Toray Industries	JK 11240979	A
	JK 11343338	4, A
Toray Industries (continued)	US 6169161	A
Toyobo	JK 02024322	A
Ube Ind	JK 01259035	A
	JK 11267405	A

Assignee	Patent Number	Chapter(s)
Union Carbide Chemicals & Plastics Technology Corporation	US 5925754	A
	US 5962680	A
Unitika	JK 10287645	A
	JK 10298162	A
	JK 11035554	A
Zimmer	DE 4316408	A
	US 5627257	A

Appendix E

PROCESS FLOW DIAGRAMS

Figure 5.1 (Sheet 1 of 4)
CAPROLACTAM FROM PHENOL BY
HYDROXYLAMINE OXIME PHOSPHATE PROCESS

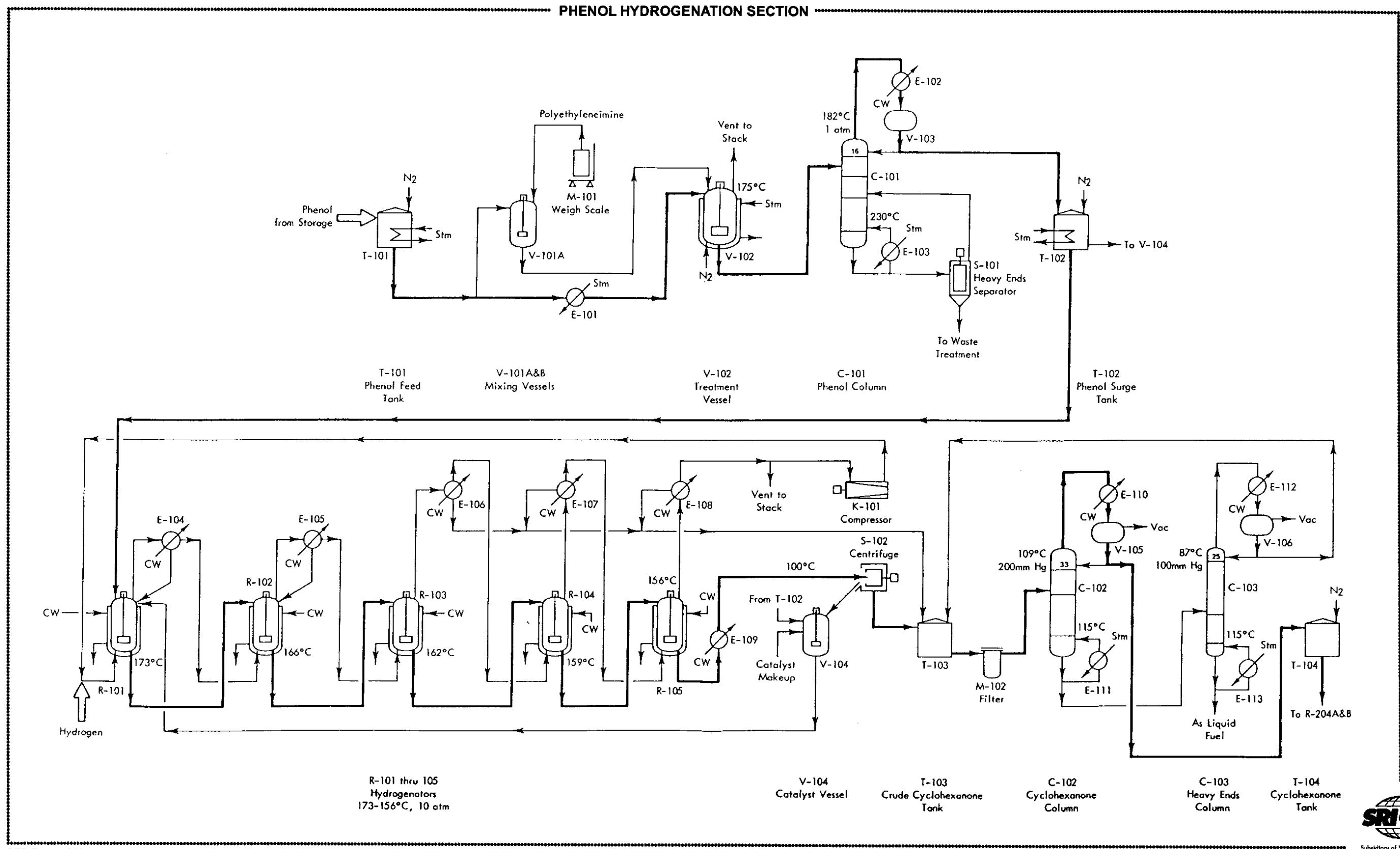


Figure 5.1 (Sheet 2 of 4)

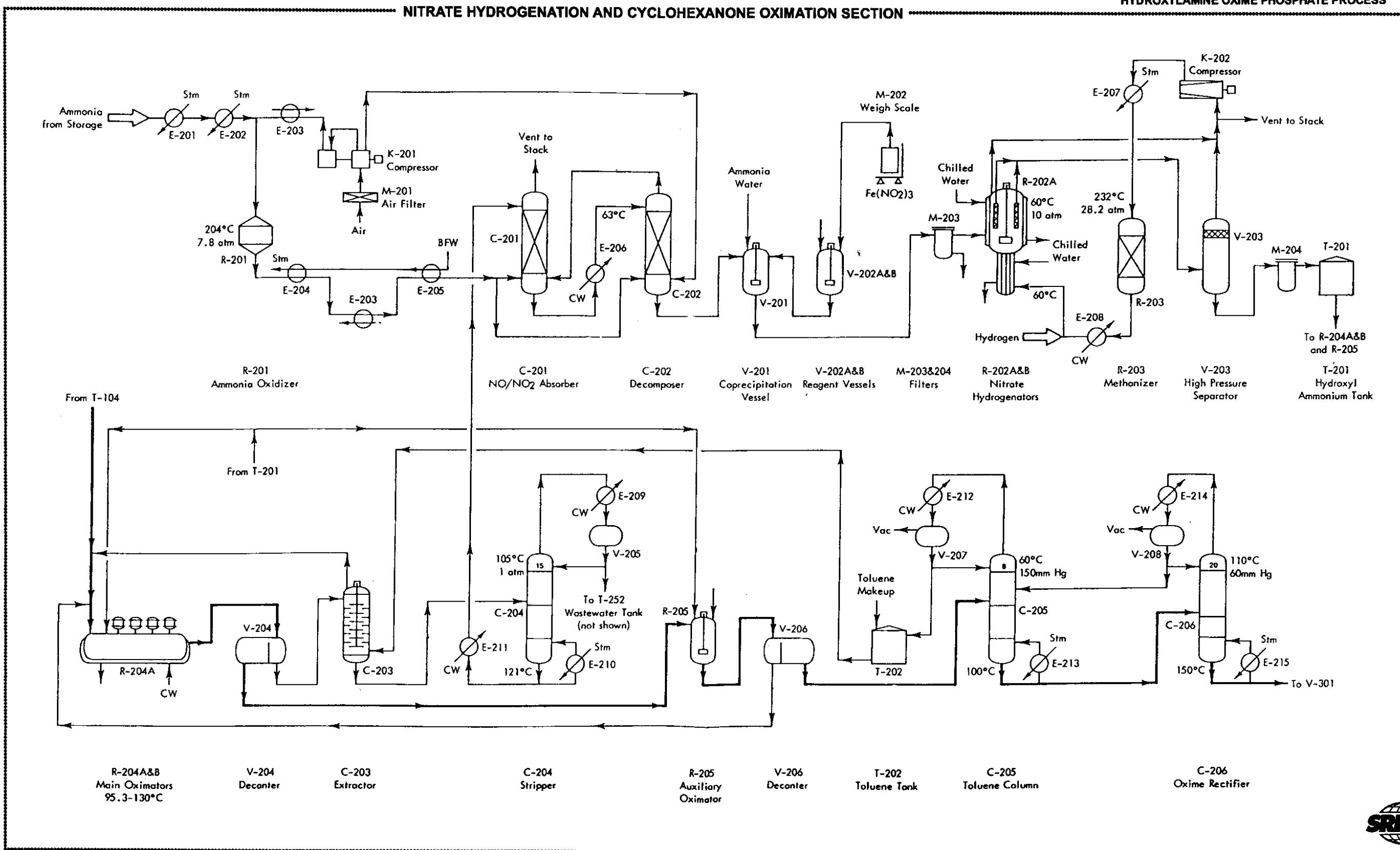
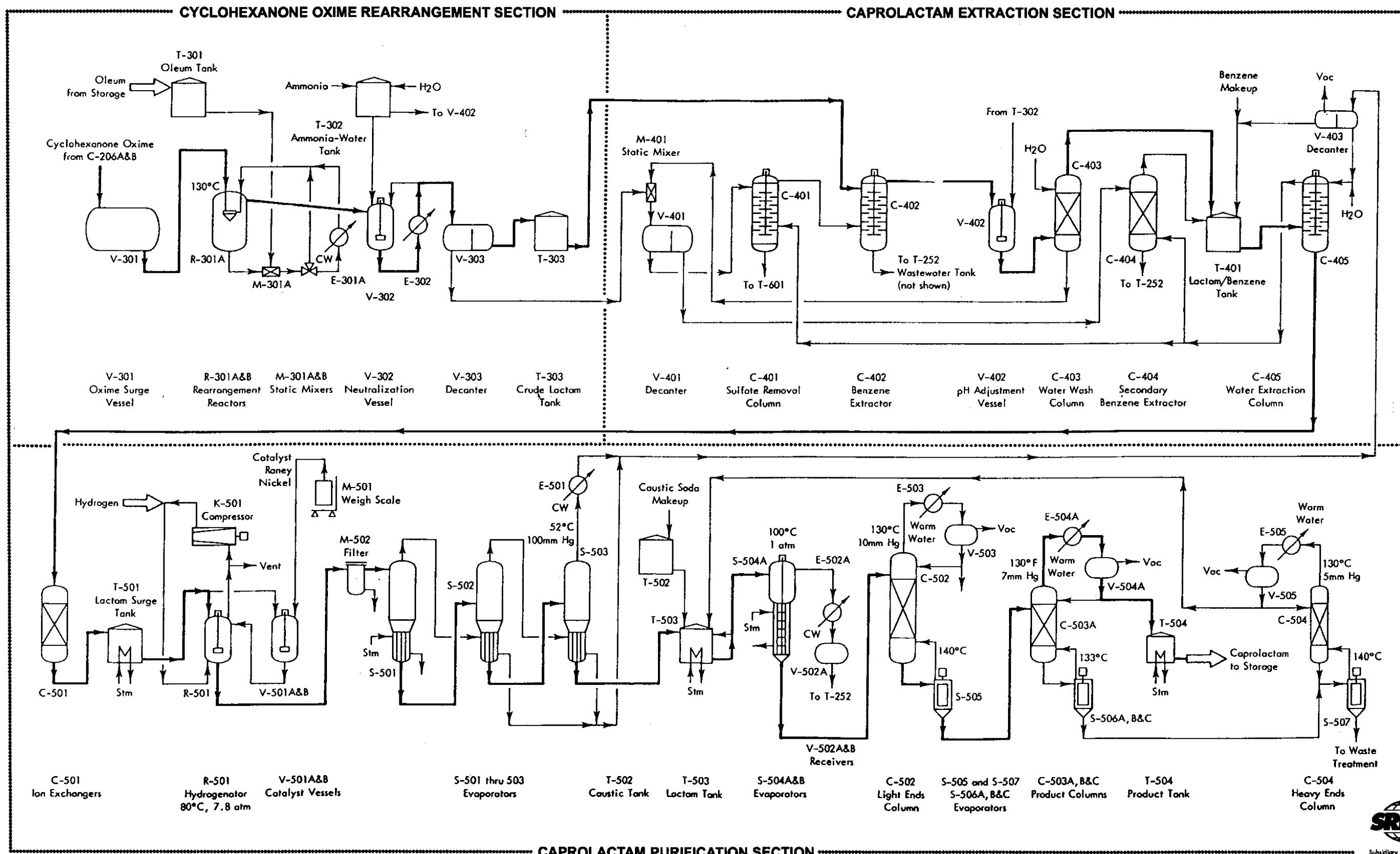
CAPROLACTAM FROM PHENOL BY
HYDROXYLAMINE OXIME PHOSPHATE PROCESS

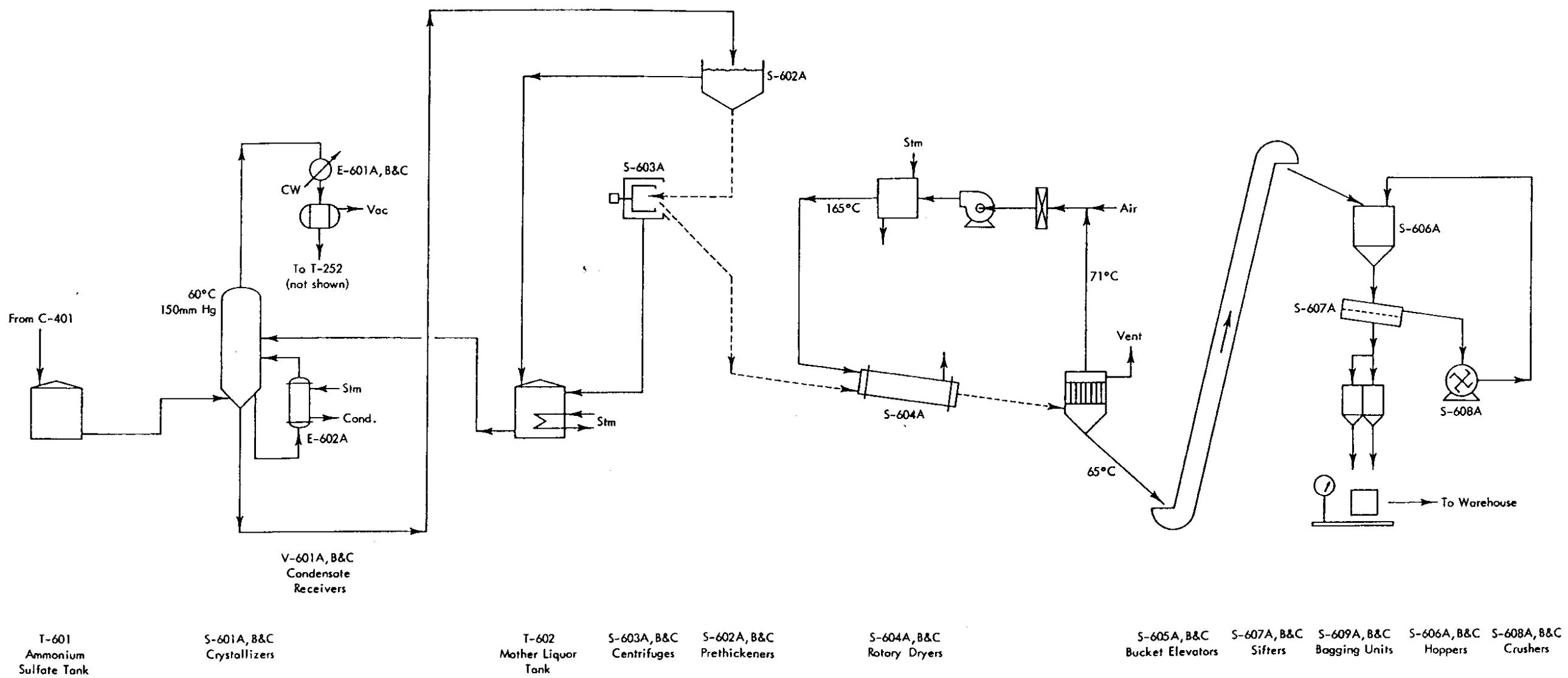
Figure 5.1 (Sheet 3 of 4)

CAPROLACTAM FROM PHENOL BY
HYDROXYLAMINE OXIME PHOSPHATE PROCESS



**CAPROLACTAM FROM PHENOL BY
HYDROXYLAMINE OXIME PHOSPHATE PROCESS**

AMMONIUM SULFATE RECOVERY SECTION



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Figure 5.2 (Sheet 1 of 4)
CAPROLACTAM FROM CYCLOHEXANE BY
NITRIC OXIDE HYDROGENATION

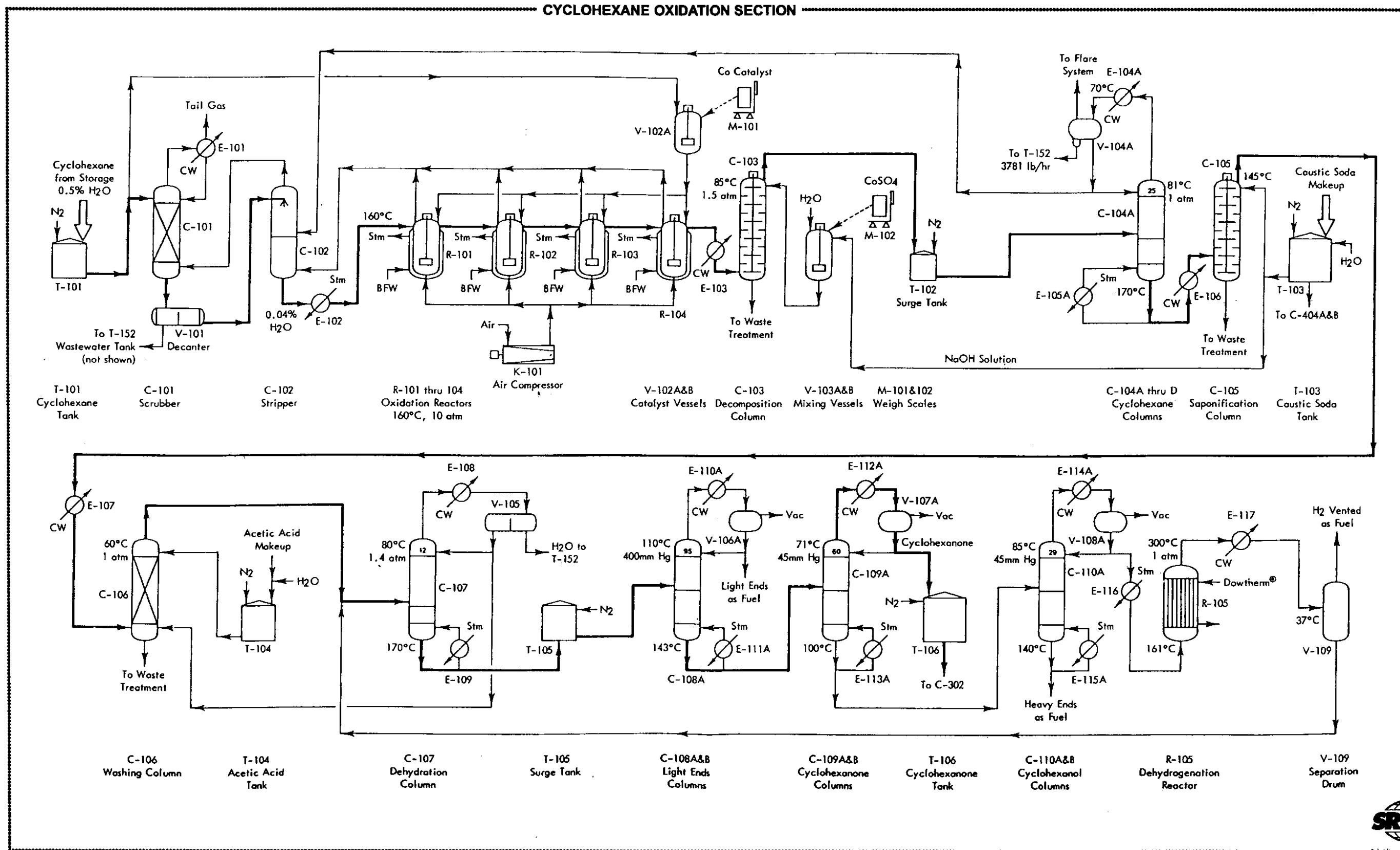
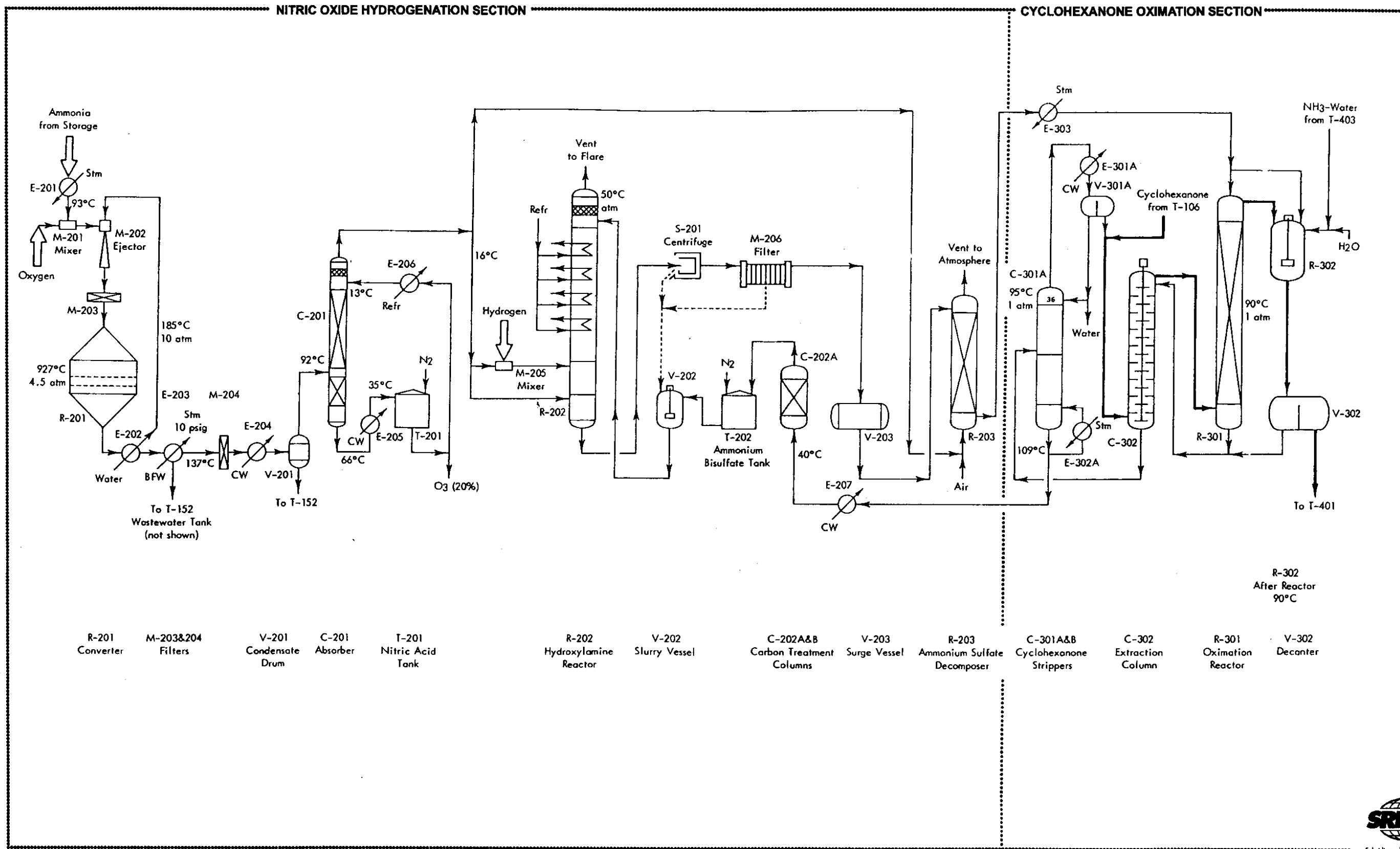


Figure 5.2 (Sheet 2 of 4)

**CAPROLACTAM FROM CYCLOHEXANE BY
NITRIC OXIDE HYDROGENATION**



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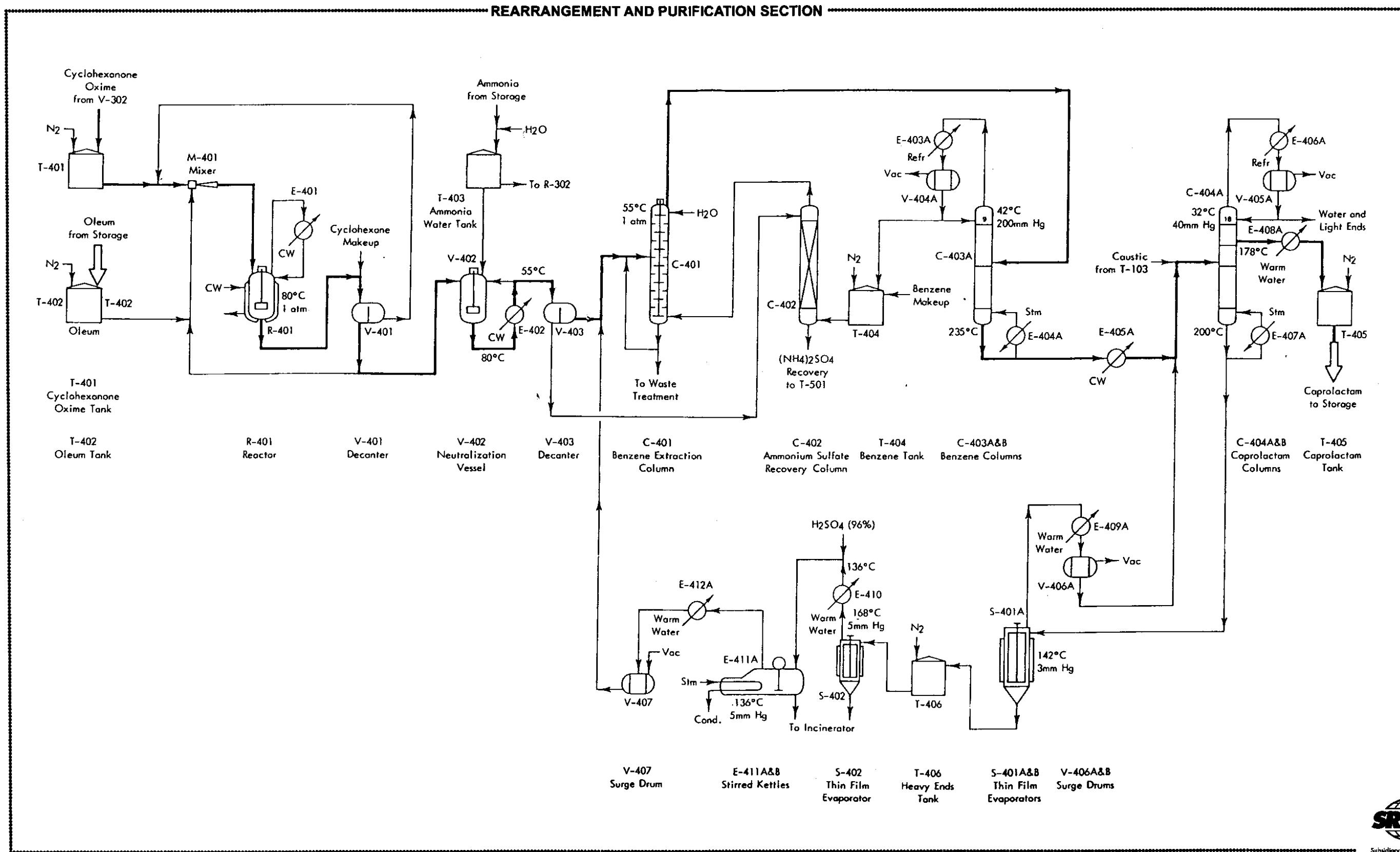
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2004

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Figure 5.2 (Sheet 3 of 4)
CAPROLACTAM FROM CYCLOHEXANE BY
NITRIC OXIDE HYDROGENATION

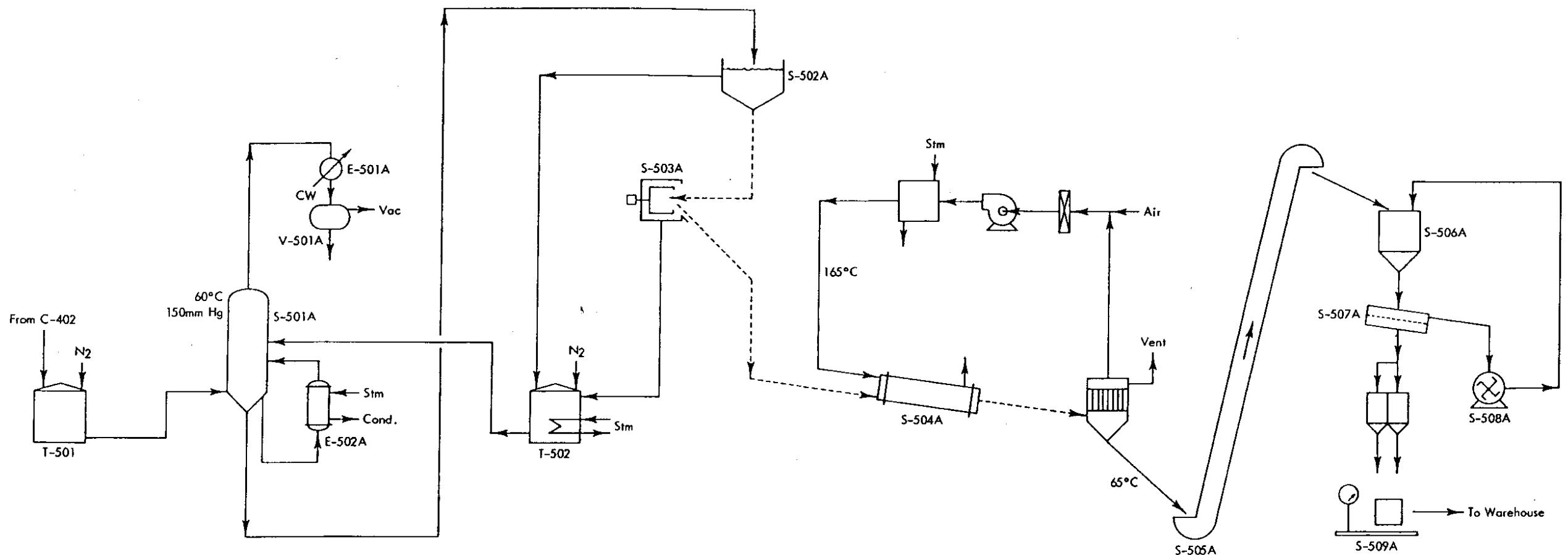
REARRANGEMENT AND PURIFICATION SECTION



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Figure 5.2 (Sheet 4 of 4)
CAPROLACTAM FROM CYCLOHEXANE BY
NITRIC OXIDE HYDROGENATION

AMMONIUM SULFATE RECOVERY SECTION



T-501
Surge Tank

S-501A,B&C
Crystallizers

V-501A,B&C
Condensate Receivers

T-502
Ammonium Sulfate
Tank

S-503A,B&C
Centrifuges

S-502A,B&C
Thickeners

S-504A,B&C
Rotary Dryers

S-505A,B&C
Bucket Elevators

S-507A,B&C
Sifters

S-509A,B&C
Bogging Units

S-506A,B&C
Hoppers

S-508A,B&C
Crushers

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Figure 5.3 (Sheet 1 of 2)
CAPROLACTAM FROM BUTADIENE

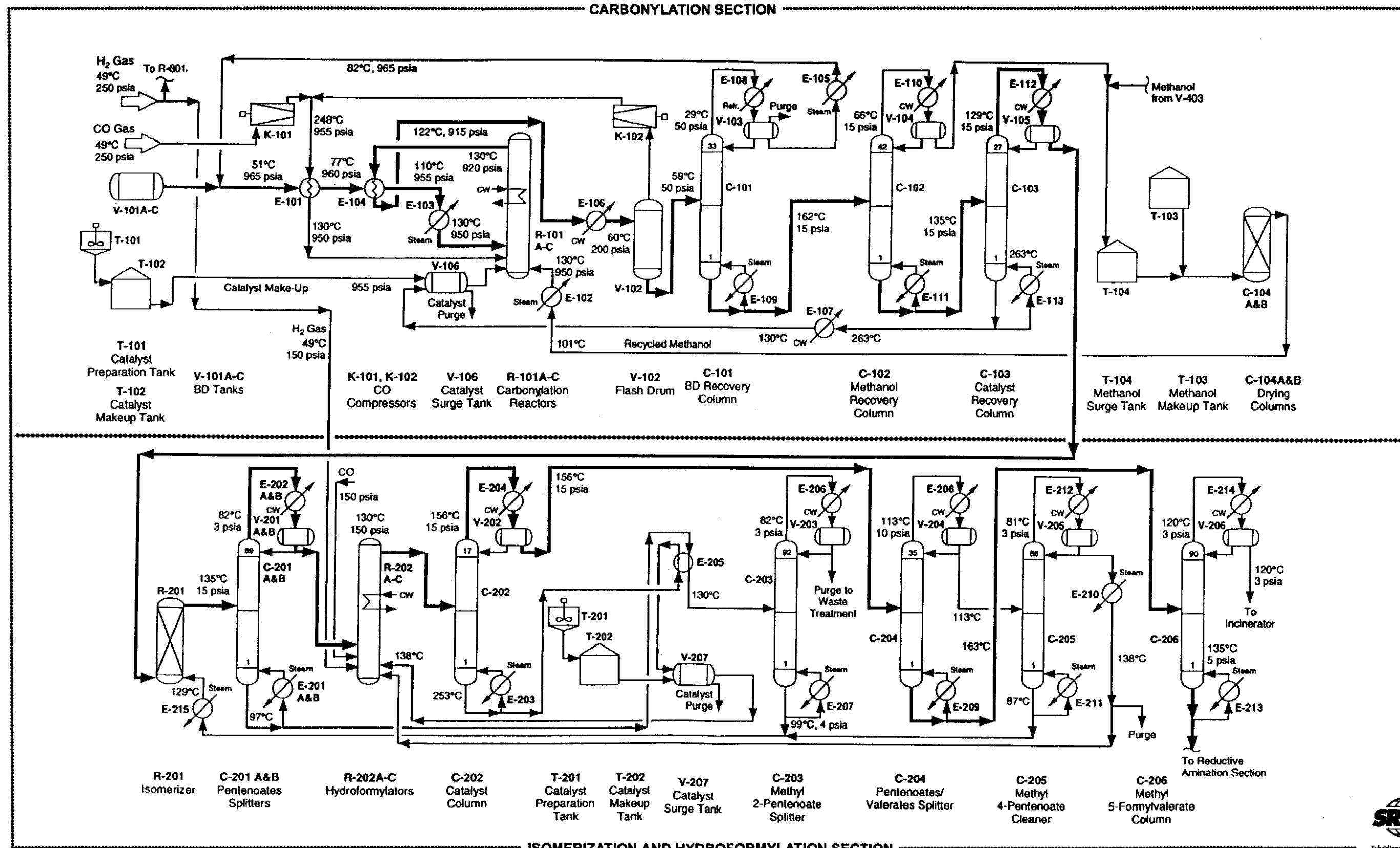
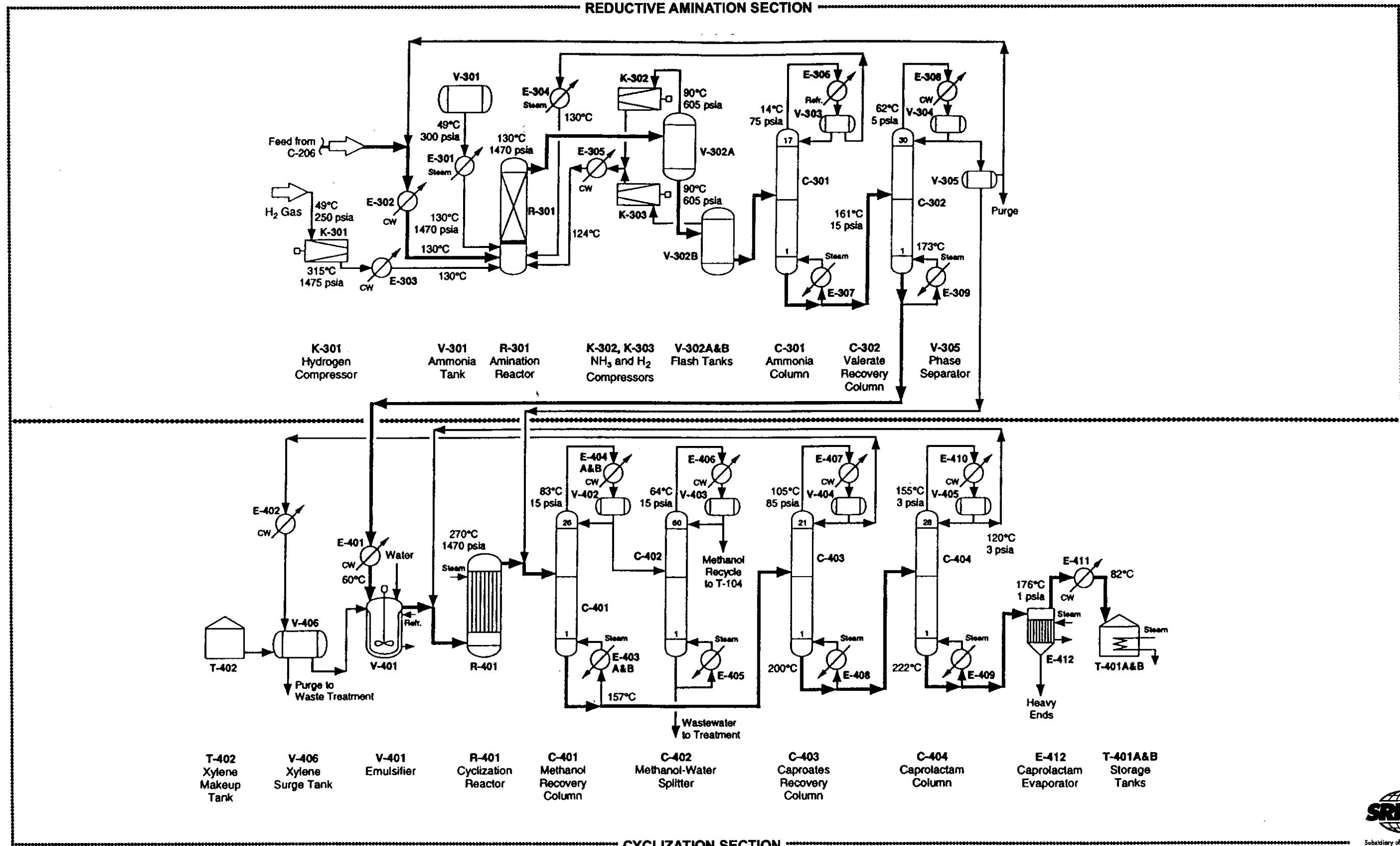


Figure 5.3 (Sheet 2 of 2)
CAPROLACTAM FROM BUTADIENE



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Figure 5.4 (Sheet 1 of 2)

CAPROLACTAM AND HMDA FROM ADIPONITRILE
BY PARTIAL HYDROGENATION

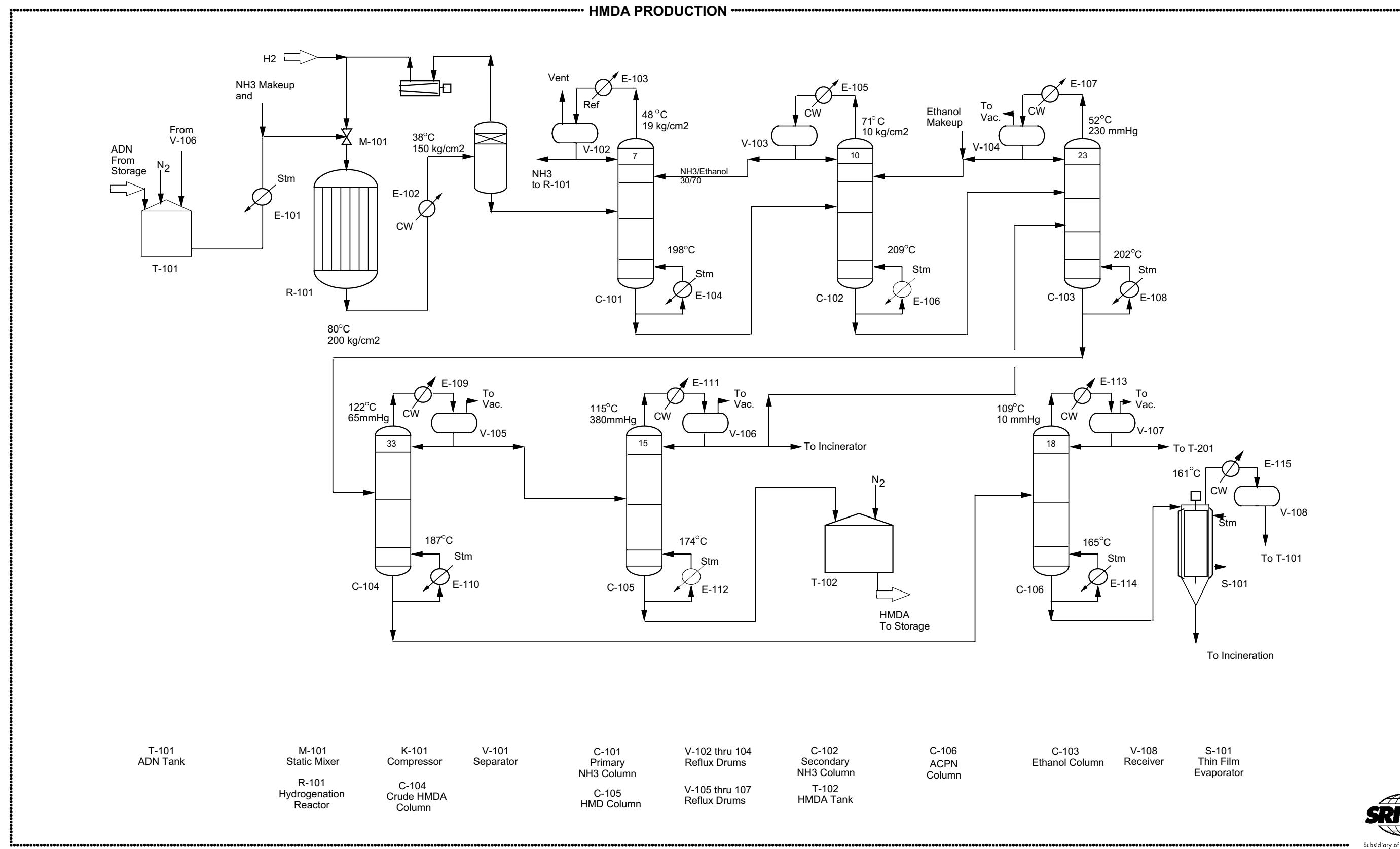
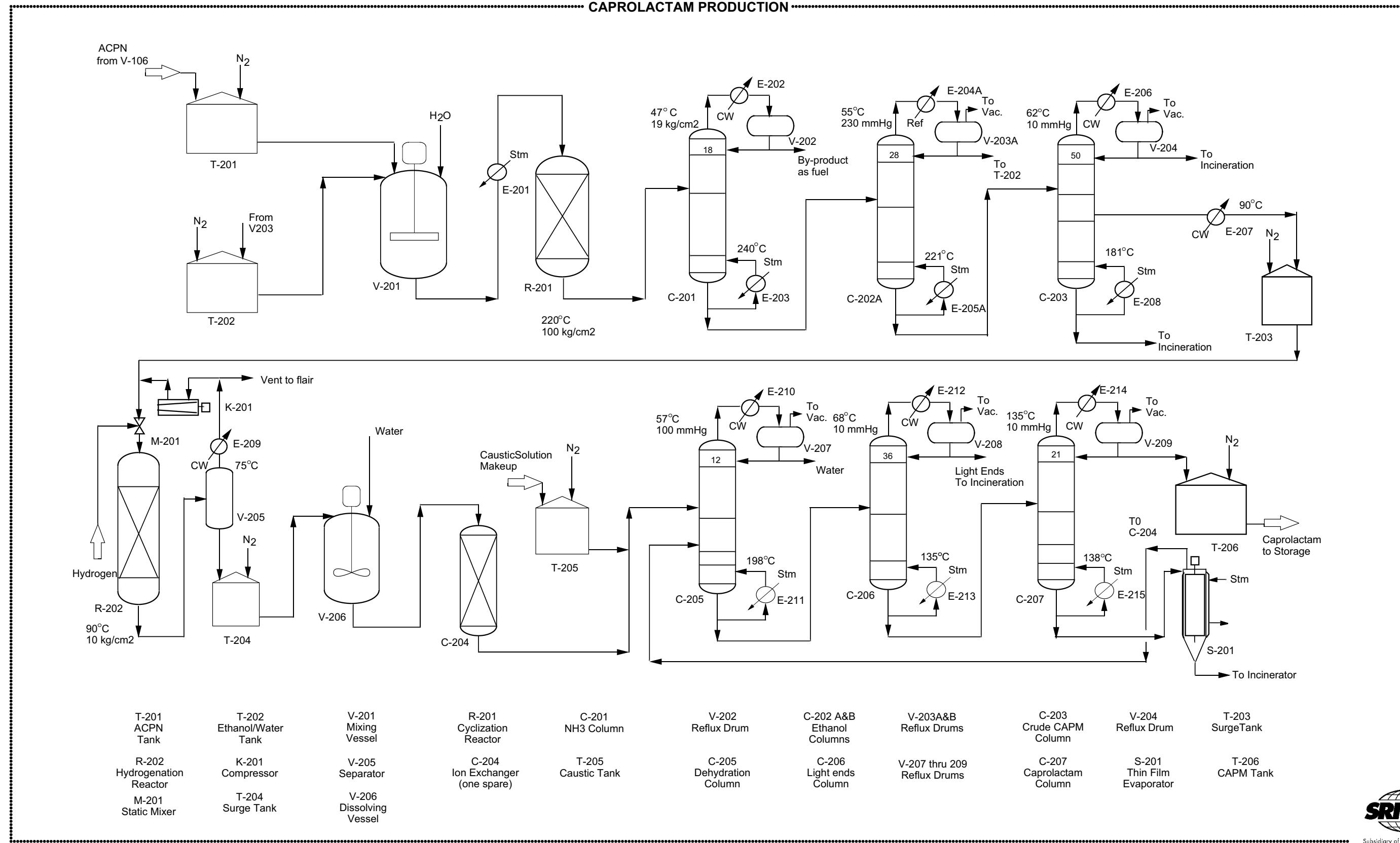


Figure 5.4 (Sheet 2 of 2)

CAPROLACTAM AND HMDA FROM ADIPONITRILE BY PARTIAL HYDROGENATION



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Figure 5.5 (Sheet 1 of 2)
CONTINUOUS PRODUCTION OF NYLON 6 CHIP

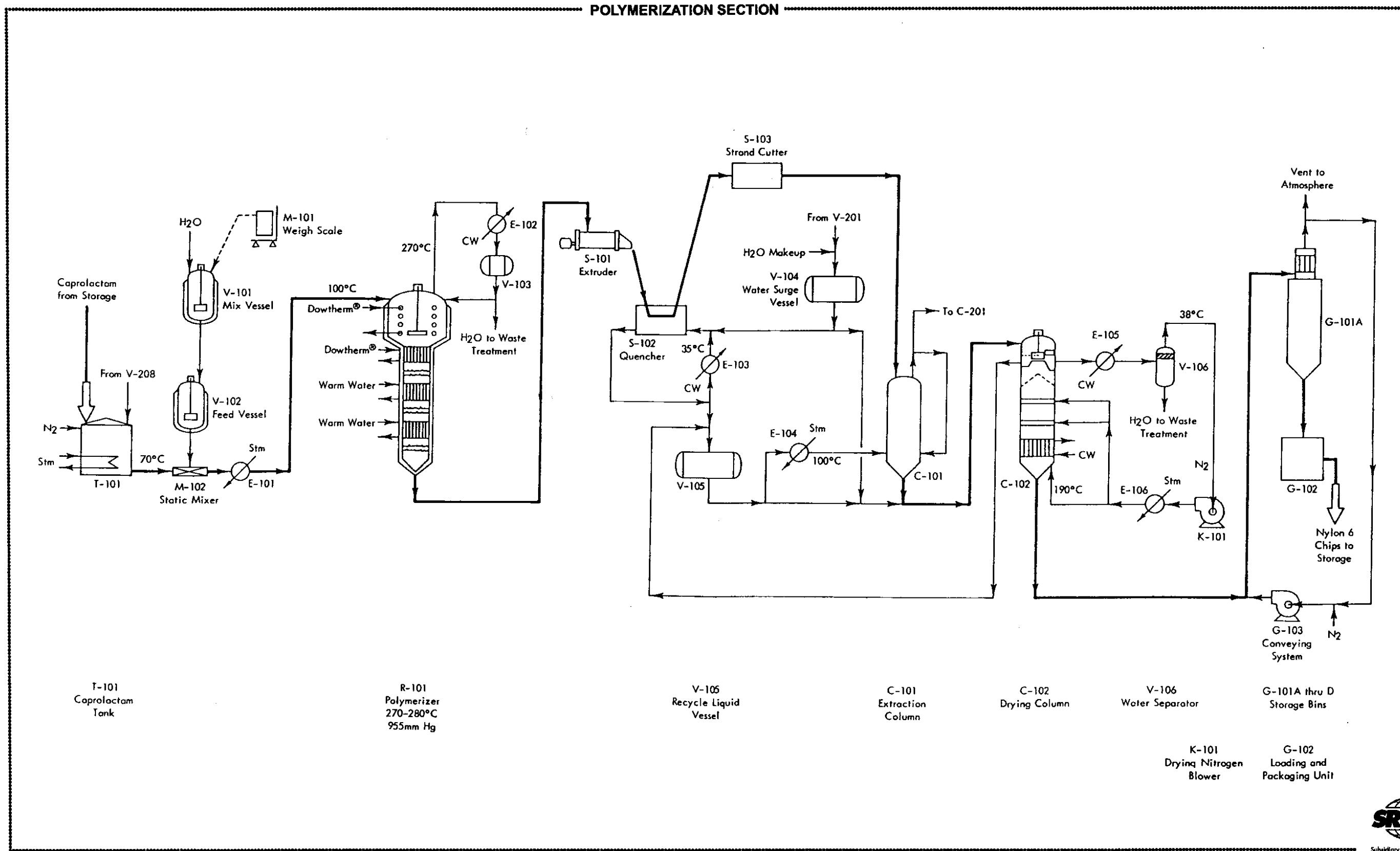


Figure 5.5 (Sheet 2 of 2)
CONTINUOUS PRODUCTION OF NYLON 6 CHIP

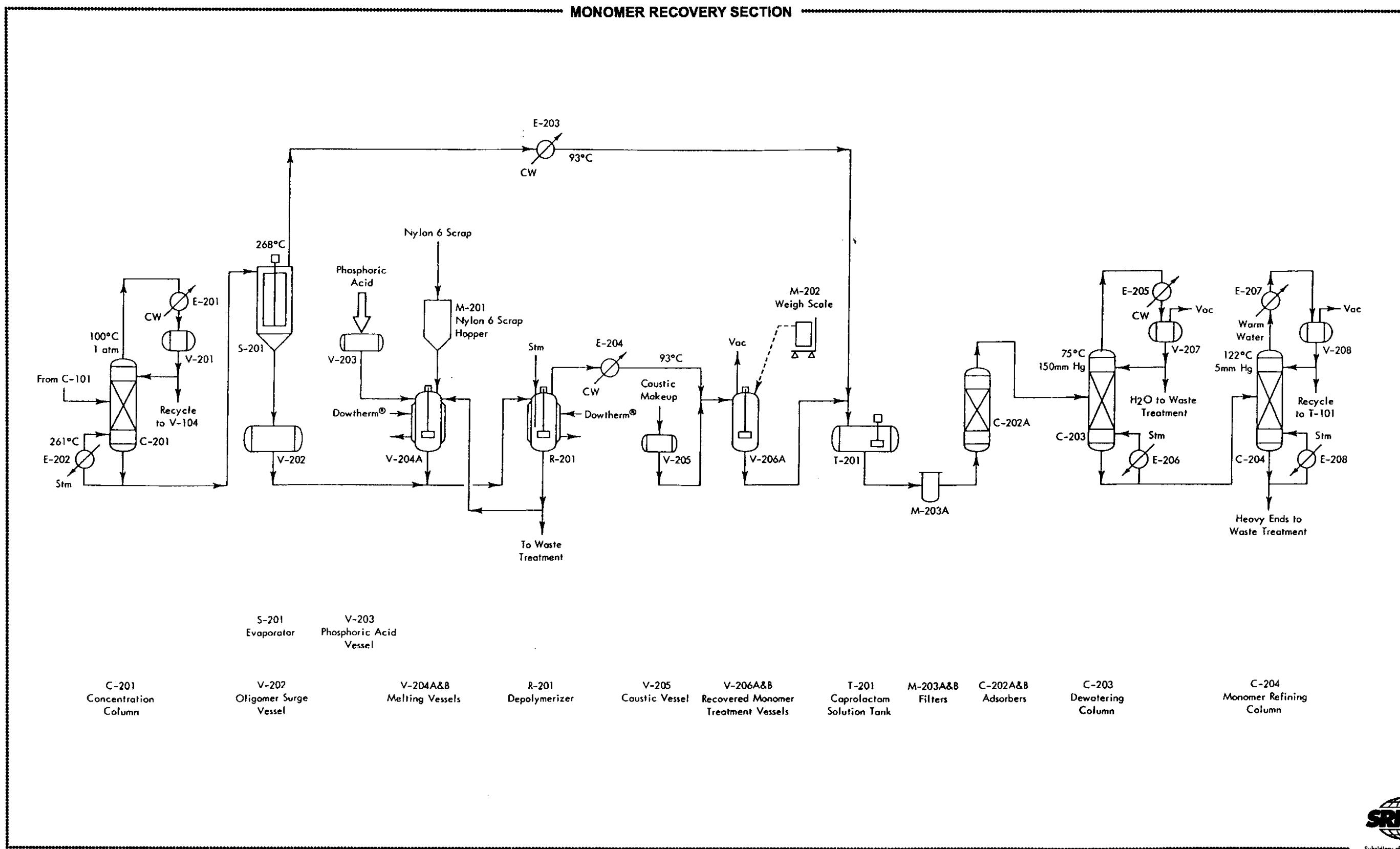
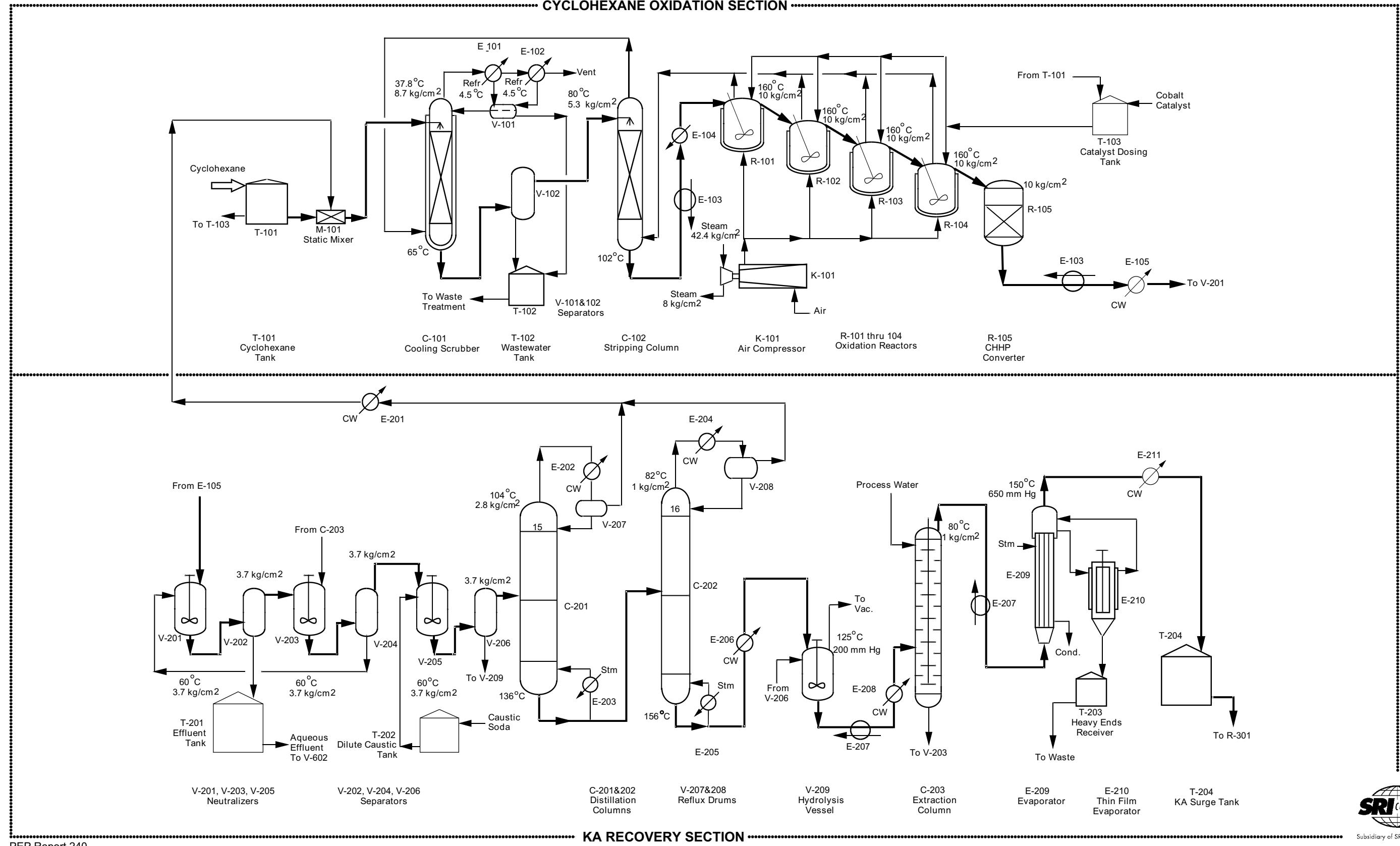


Figure 6.1 (Sheet 1 of 3)

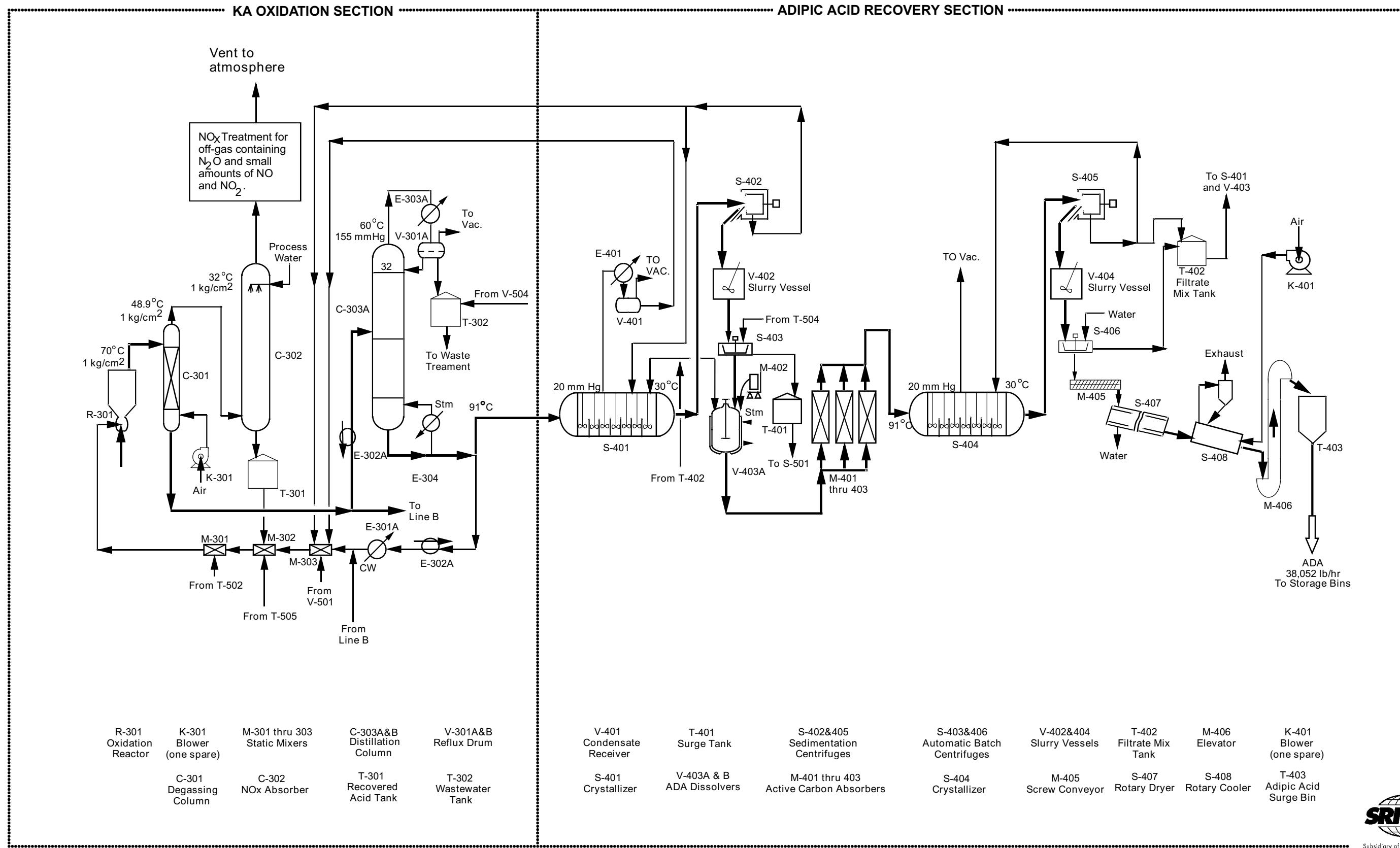
**ADIPIC ACID FROM CYCLOHEXANE
BY OXIDATION PROCESS**



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Figure 6.1 (Sheet 2 of 3)
ADIPIC ACID FROM CYCLOHEXANE
BY OXIDATION PROCESS



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Figure 6.1 (Sheet 3 of 3)
ADIPIC ACID FROM CYCLOHEXANE
BY OXIDATION PROCESS

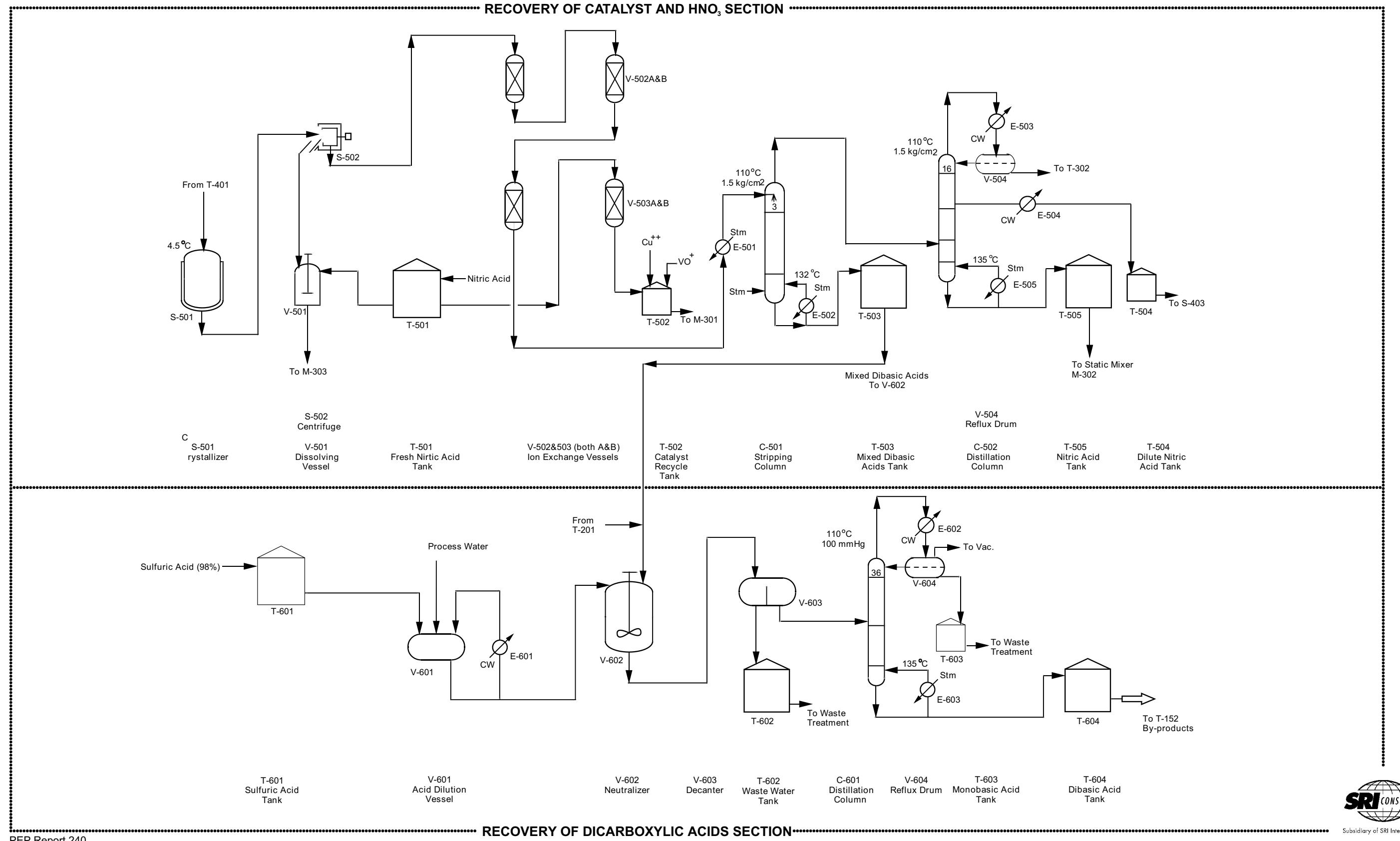
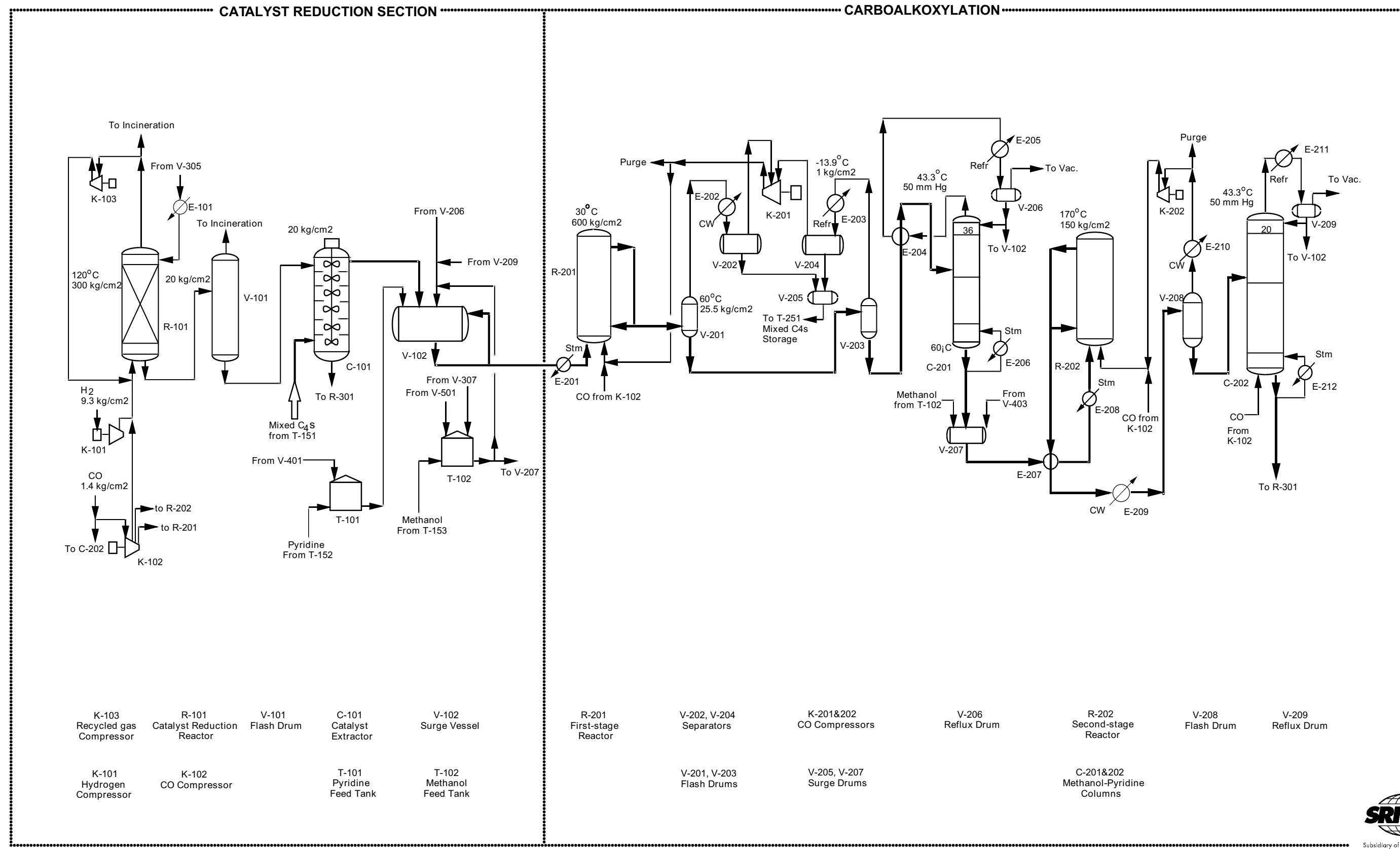


Figure 6.2 (Sheet 1 of 3)
ADIPIC ACID FROM BUTADIENE
BY CARBOALKOXYLATION



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Figure 6.2 (Sheet 2 of 3)
ADIPIC ACID FROM BUTADIENE
BY CARBOALKOXYLATION

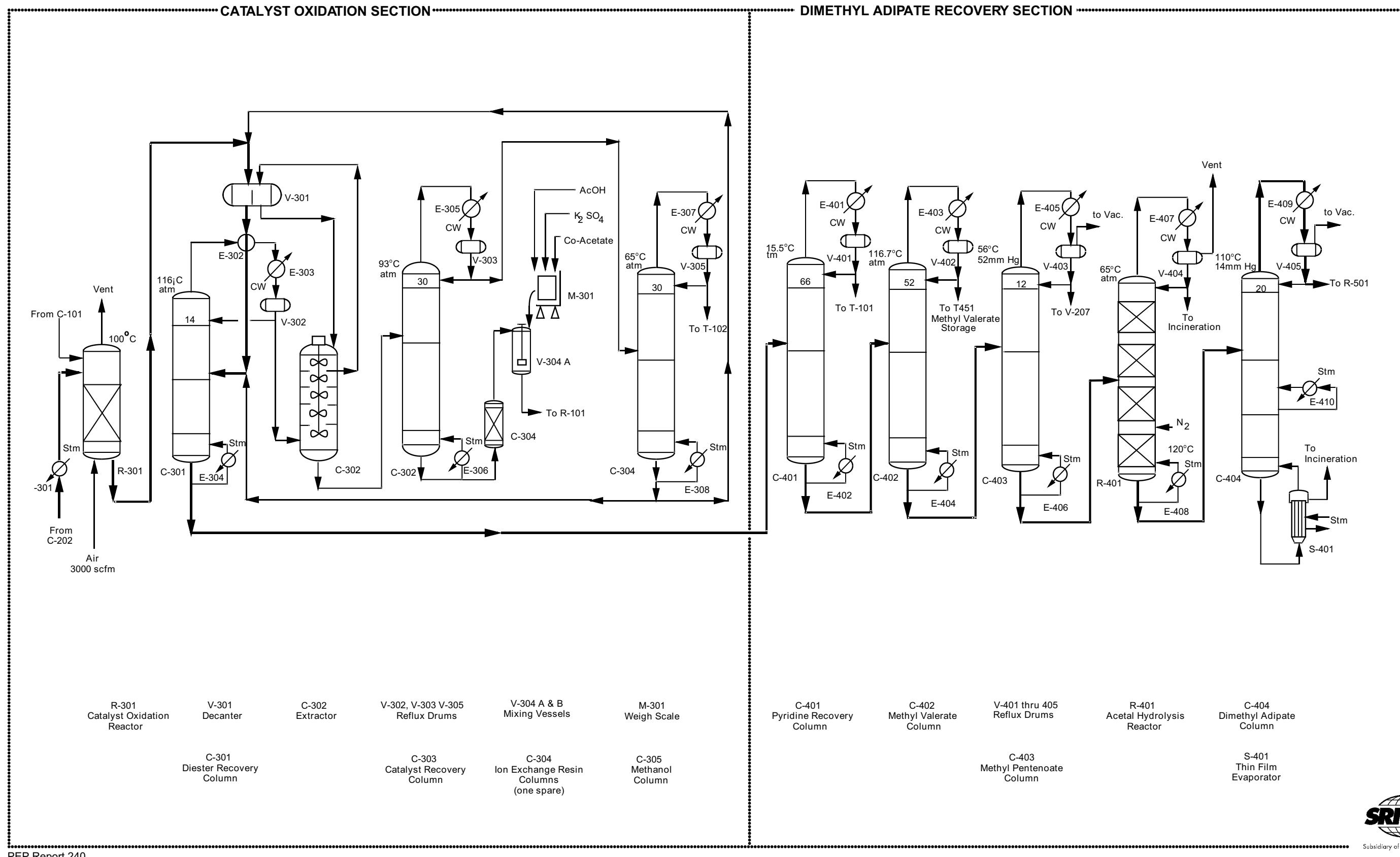
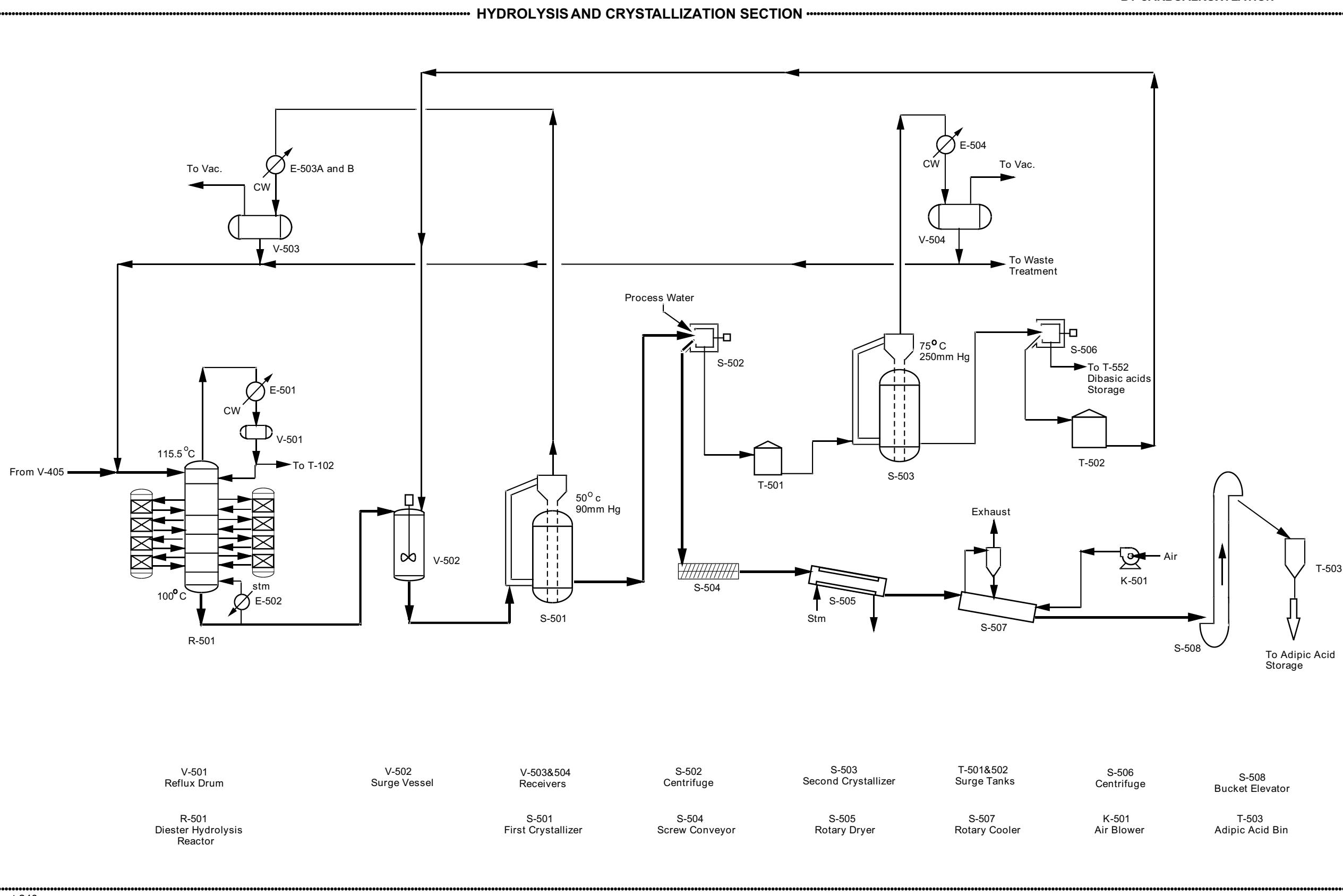


Figure 6.2 (Sheet 3 of 3)
ADIPIC ACID FROM BUTADIENE
BY CARBOALKOXYLATION



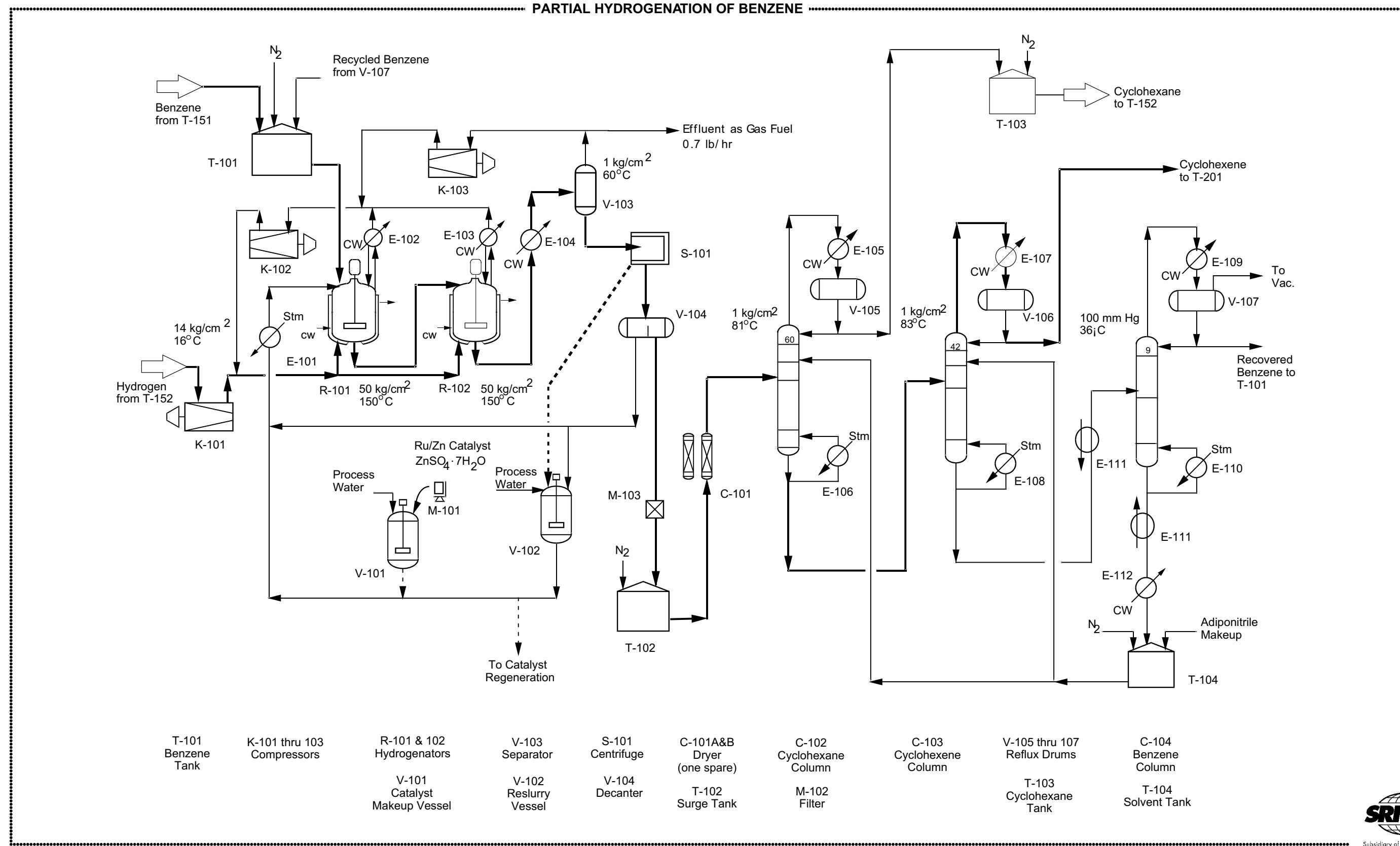
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Figure 6.3 (Sheet 1 of 2)

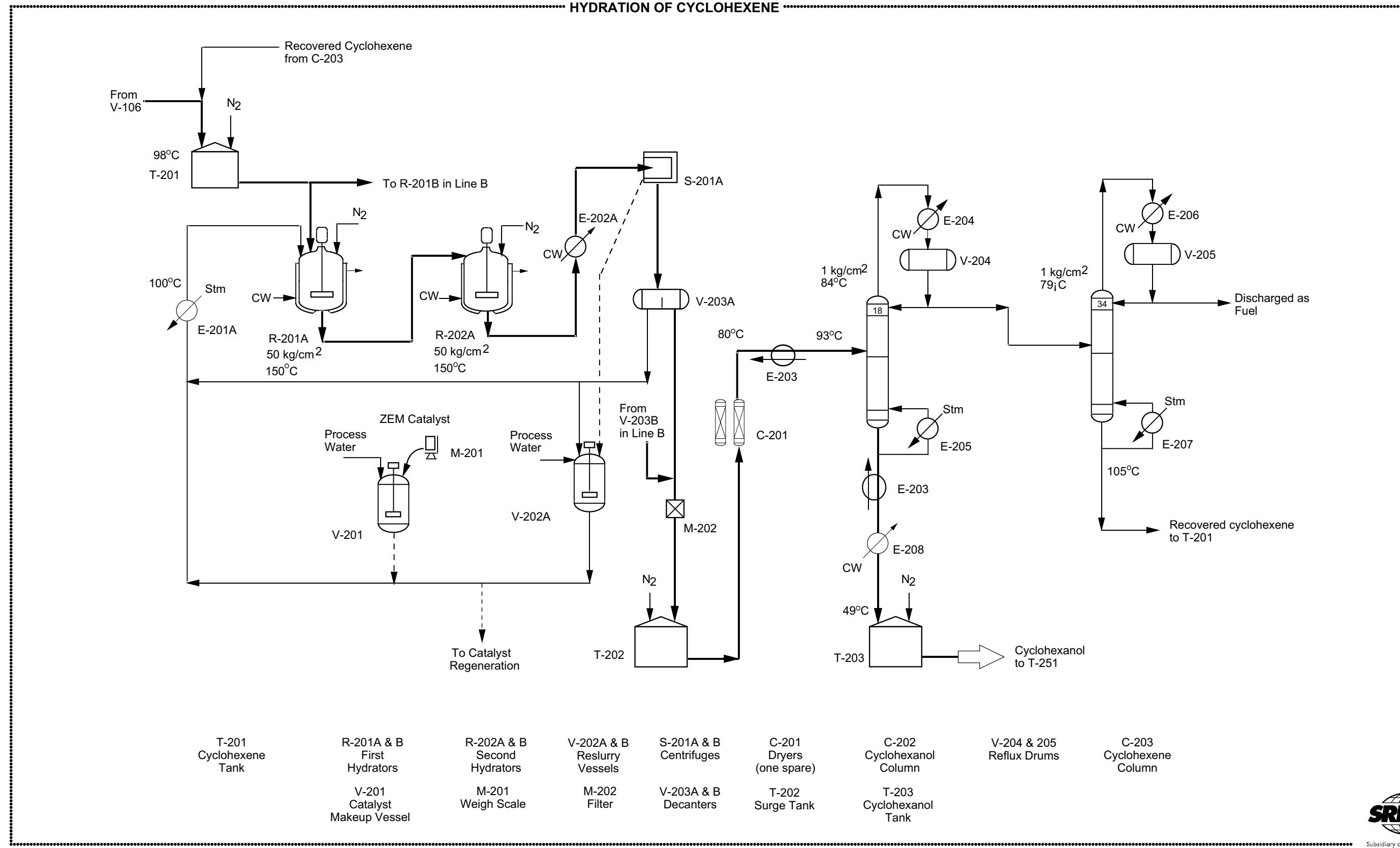
CYCLOHEXANOL FROM BENZENE BY PARTIAL HYDROGENATION AND HYDRATION



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Figure 6.3 (Sheet 2 of 2)

CYCLOHEXANOL FROM BENZENE BY PARTIAL HYDROGENATION AND HYDRATION



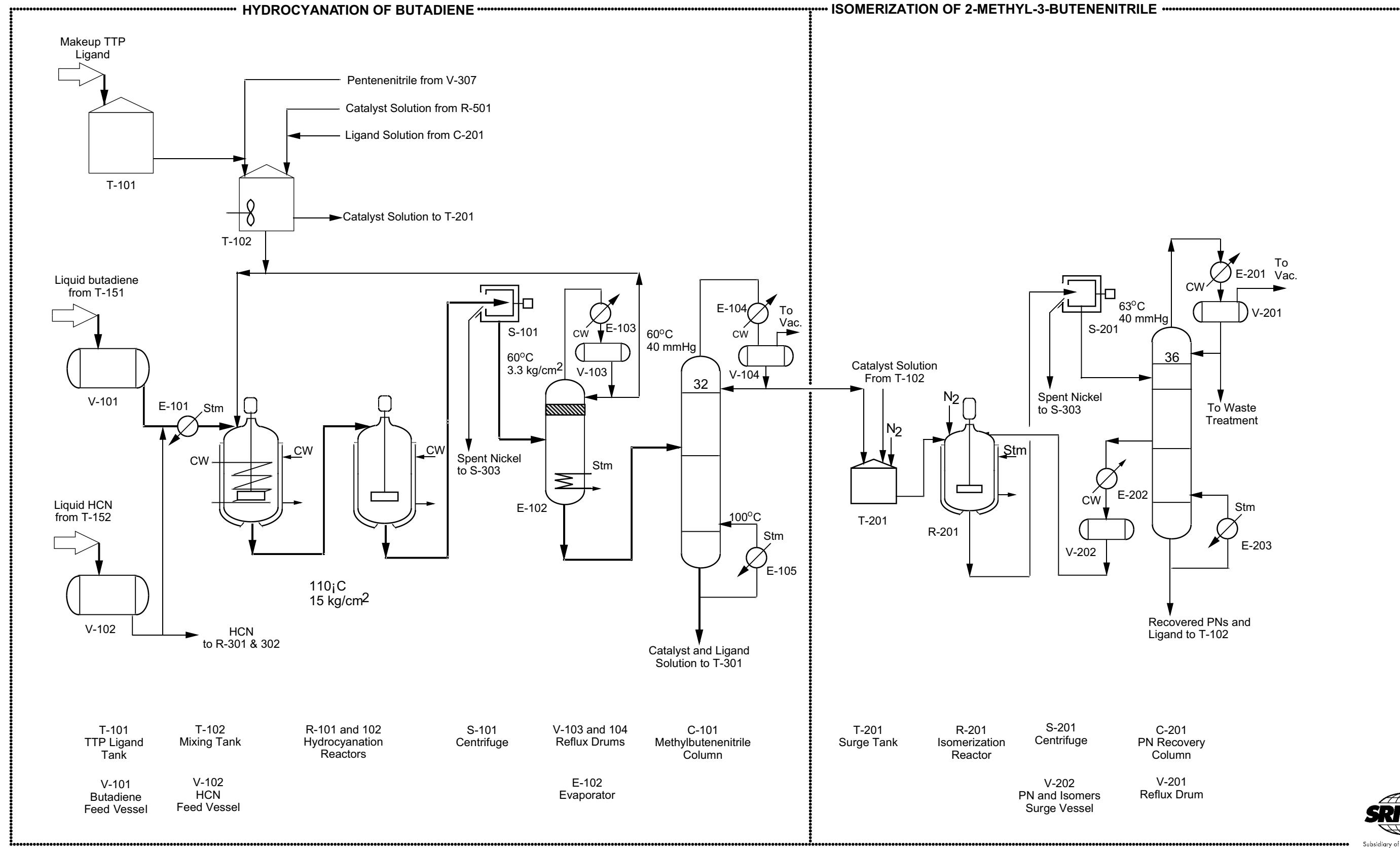
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Figure 6.4 (Sheet 1 of 4)

**HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION**



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Figure 6.4 (Sheet 2 of 4)

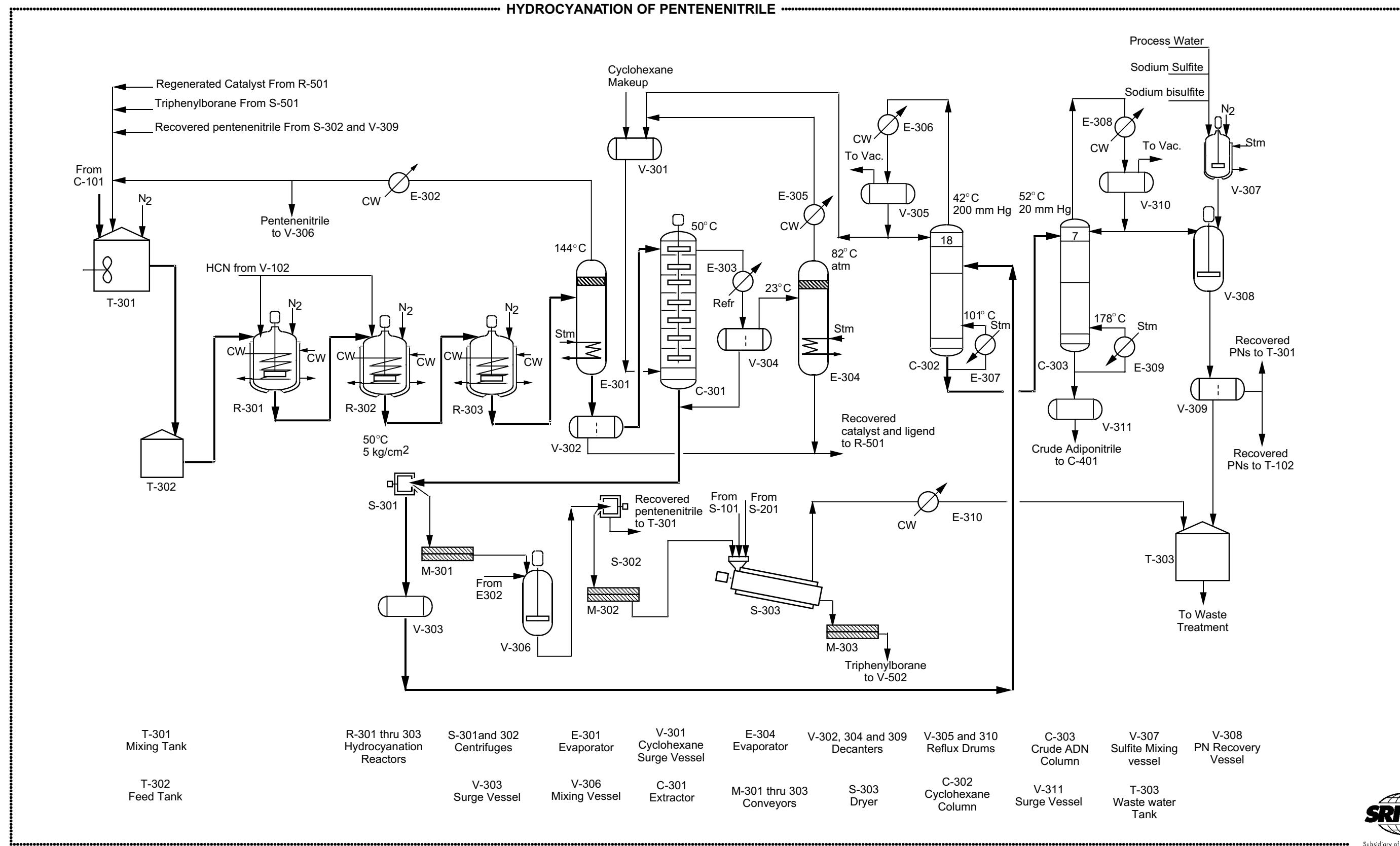
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

Figure 6.4 (Sheet 3 of 4)
HEXAMETHYLENEDIAMINE FROM BUTADIENE
VIA ADIPONITRILE BY HYDROCYANATION

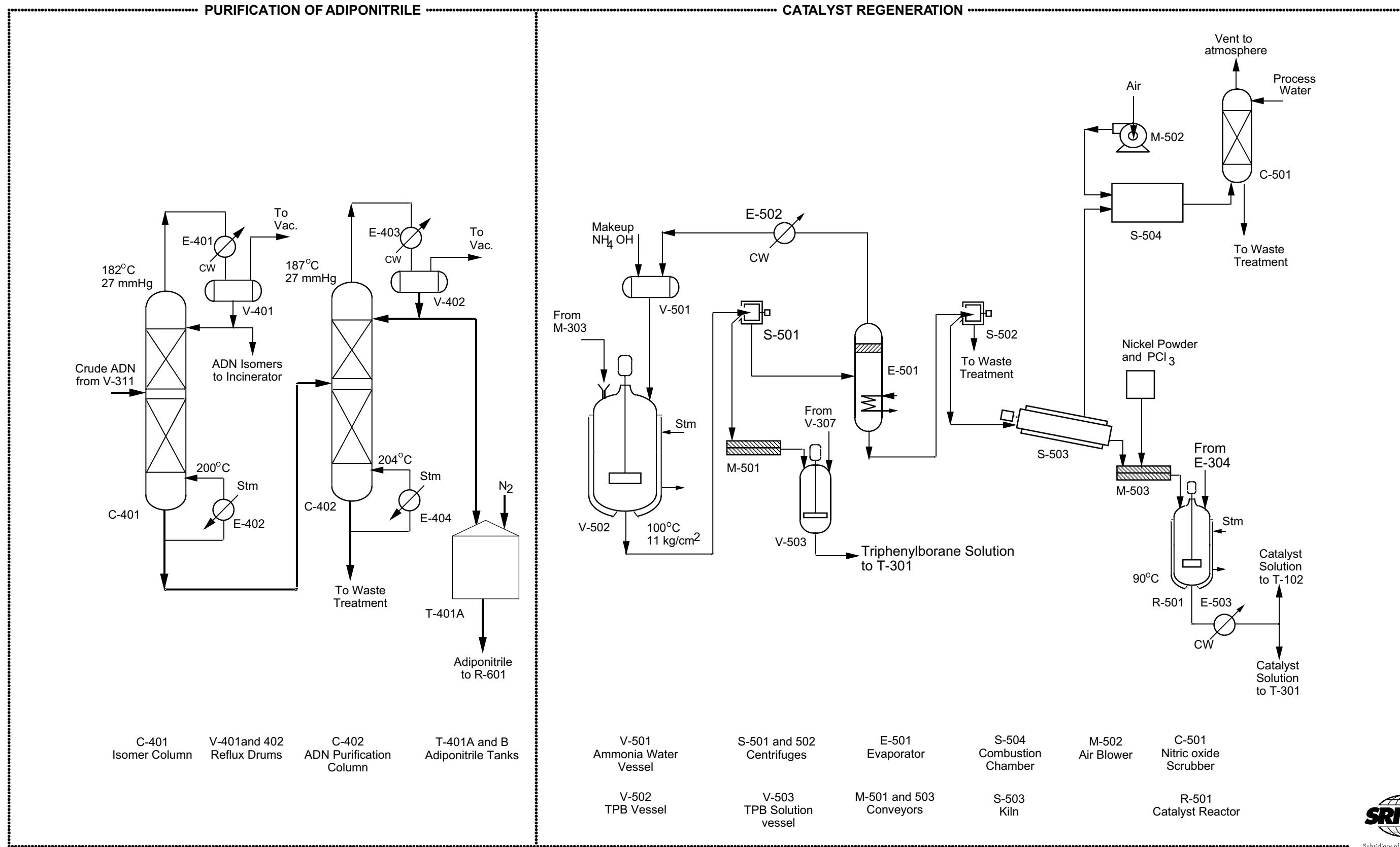
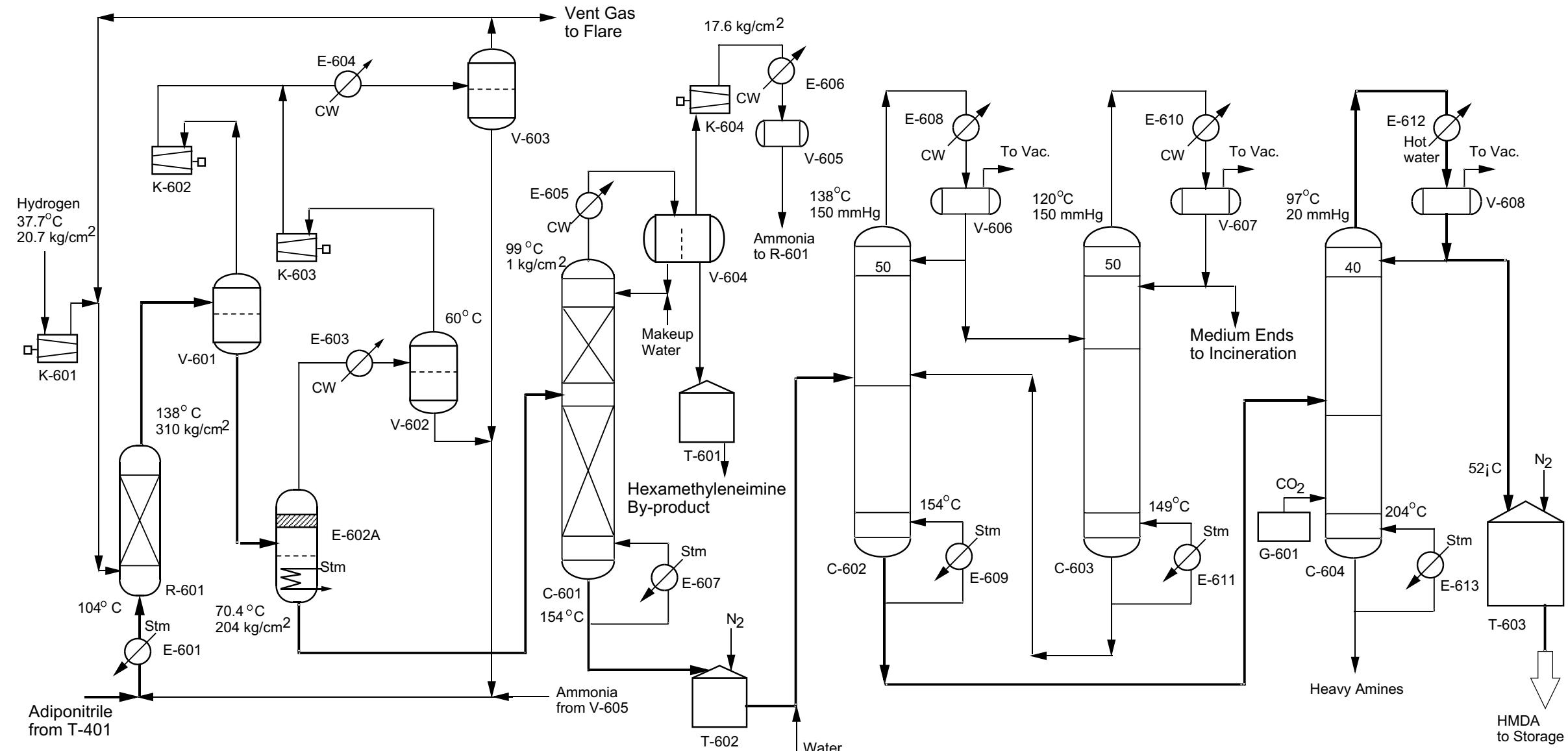


Figure 6.4 (Sheet 4 of 4)

HEXAMETHYLEDIAMINE FROM BUTADIENE VIA ADIPONITRILE BY HYDROCYANATION

..... HYDROGENATION OF ADIPONITRILE



K-601 thru 604
Hydrogen Compressors
(each has one spare)

R-601
Hydrogena

V-601 thru 603
Separators

E-602A and B Evaporators

V-604
Reflux Dr

C-601
Imine Stripper

T-601
Hexamethyleneimi

T-60
Surge

K-604
Ammonia
Compresso

V-605
Received

V-606 thru 608
Reflux Drums

C-603
Medium Bo
Stripper

G-601
Carbon Dioxide Unit

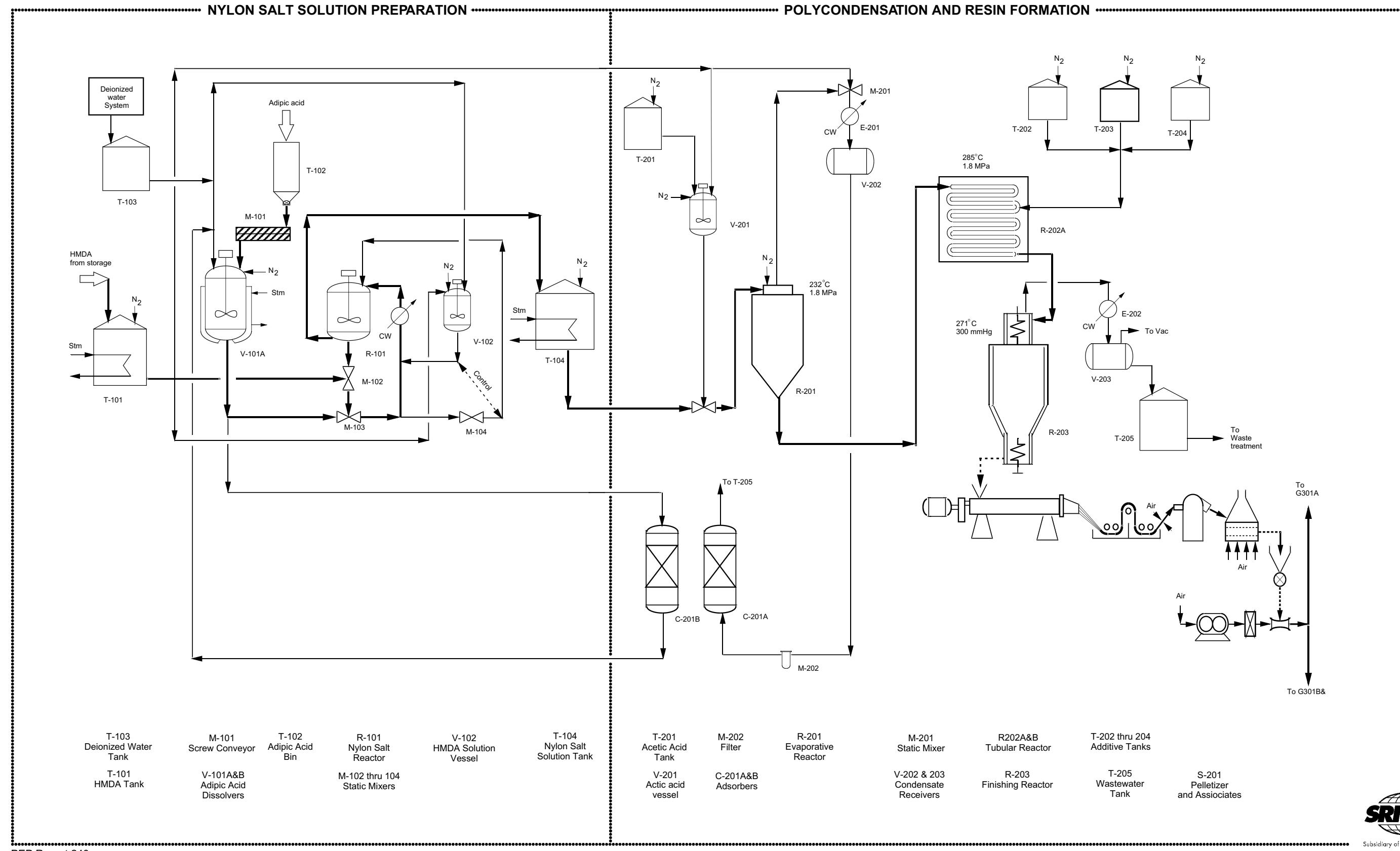
C-604
HMDA Column

T-603
HMDA Tank



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Figure 6.5 (Sheet 1 of 2)
NYLON 66 RESIN BY CONTINUOUS PROCESS



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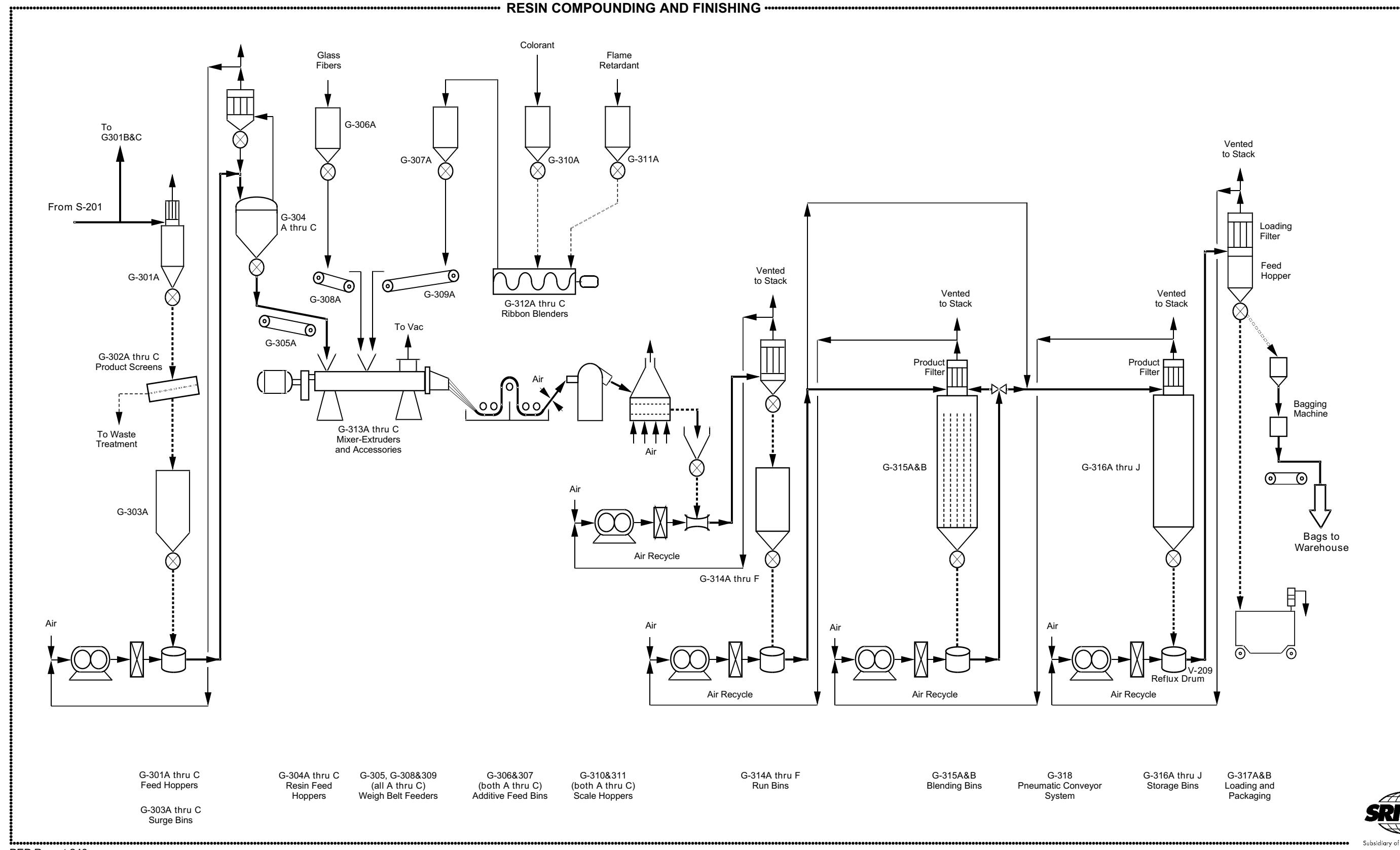


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Figure 6.5 (Sheet 2 of 2)
NYLON 66 RESIN BY CONTINUOUS PROCESS



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