

Supporting Information

Economically-feasible Production of a Nylon Monomer using Raney Catalysts

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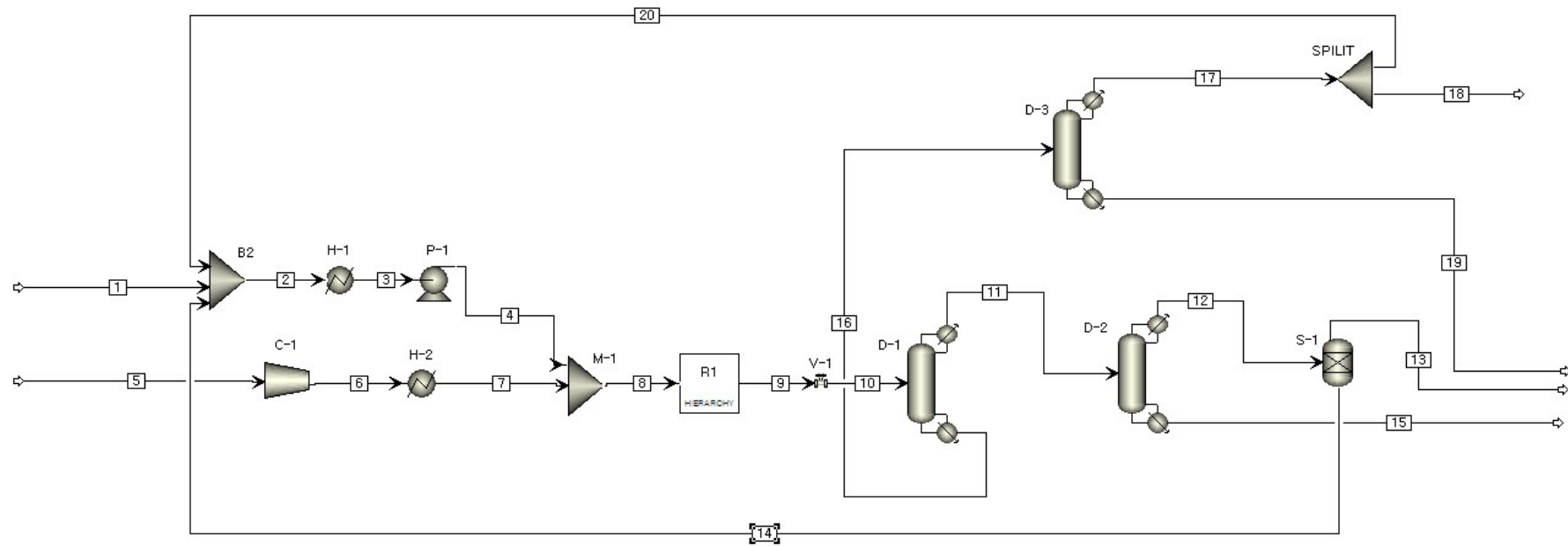


Figure S1. Detailed stream data associated with Figure 6 in the main text

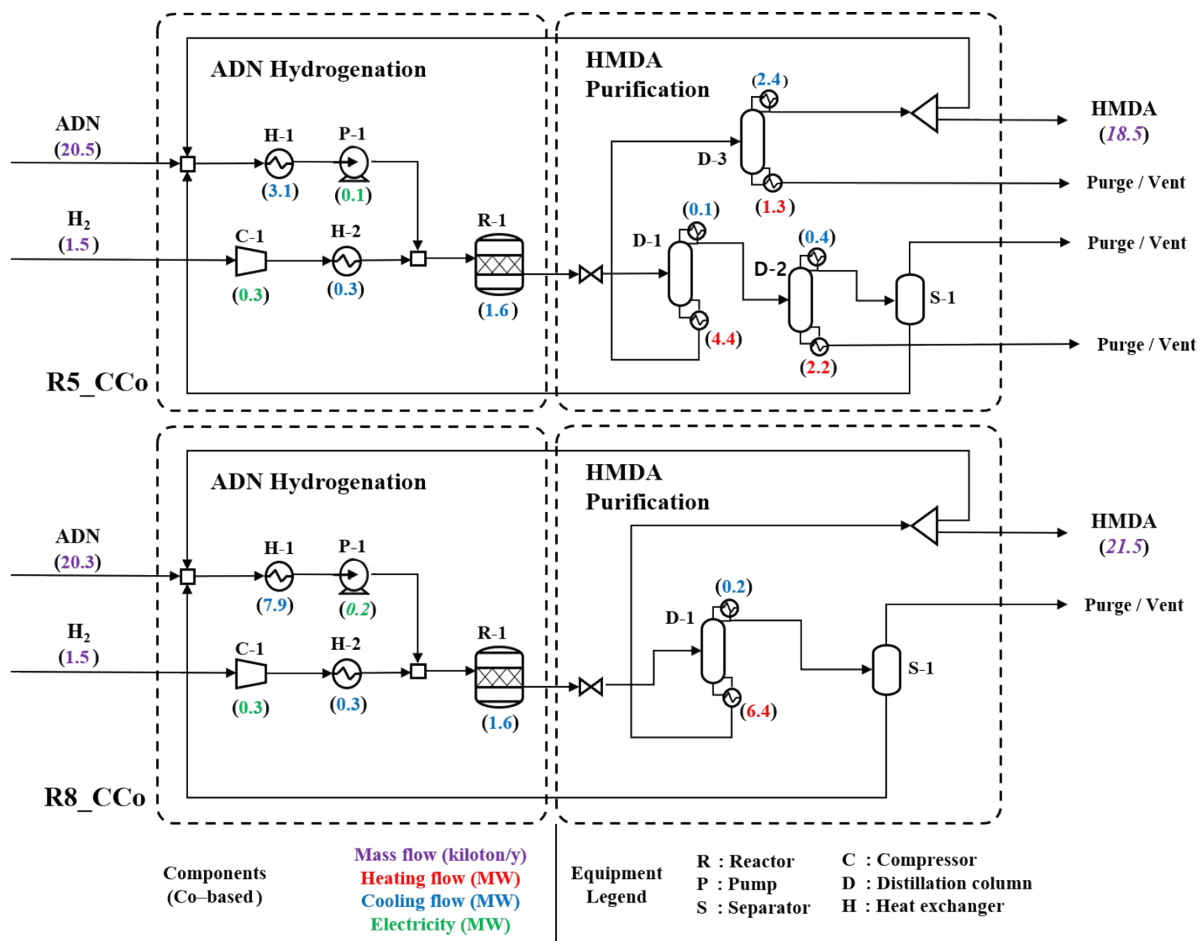
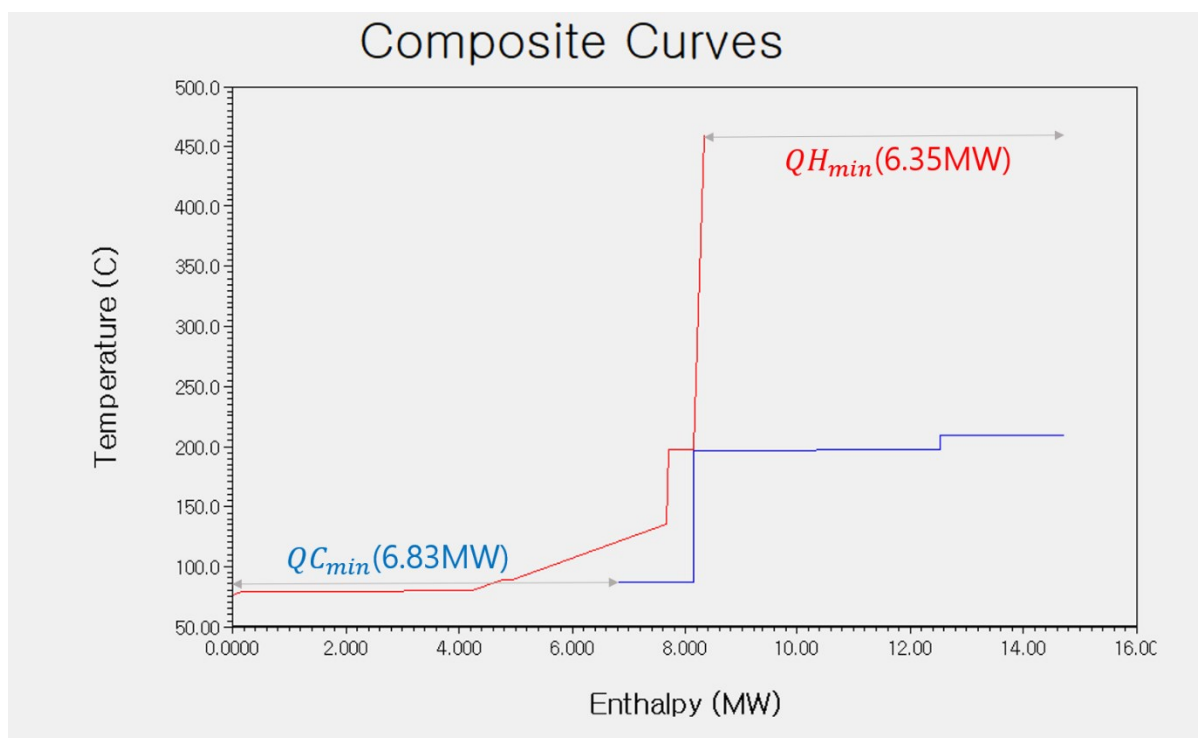


Figure S2. Process flow diagram for HMDA production from ADN (Case CCo)



No.	stream		Inlet T [K]	Outlet T [K]	MW
1	2→3	↙	136.8	77.0	-3.5
2	8→9	↙	80.5	80.0	-1.6
3	10→11	↙	91.0	90.5	-0.1
4	10→16	↗	197.4	197.9	4.4
5	6→7	↙	460.6	80.0	-0.3
6	11→12	↙	198.9	198.4	-0.4
7	11→15	↗	209.9	210.4	2.2
8	16→17	↙	81.3	80.8	-2.4
9	16→19	↗	87.4	87.9	1.3

Figure S3. Composite curve for the process (obtained using ASPEN Energy Analyzer); minimum temperature difference (ΔT_{min}) is 10 °C. The estimated total minimum area requirement (A_{min}) is Case R5_CNi:2705 m². The total minimum hot/cold utility requirement (Q_{Hmin}/Q_{Cmin}) is 6.35MW/6.83MW

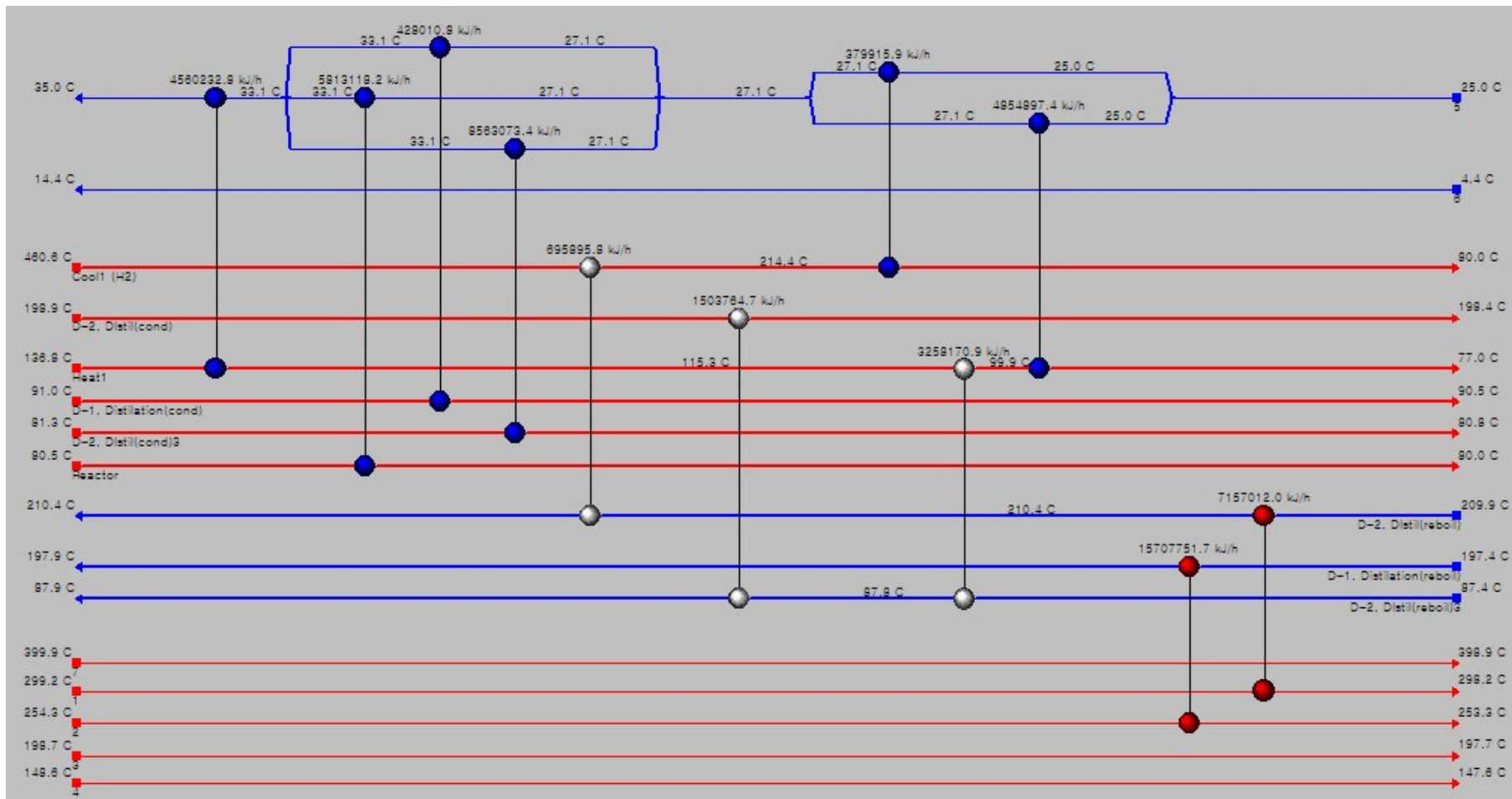


Figure S4. Grid diagram for HMDA production from ADN

Table S1. Analysis conditions of the GC-FID used in this study

	Syringe Type	10 μ L glass fixed needle
Injector setting	Split ratio	10:1
	Injection Volume (μ L)	1
	Inlet temperature ($^{\circ}$ C)	230
	Detector temperature ($^{\circ}$ C)	250
GC-FID setting	H ₂ flow rate (mL/min)	30
	Argon flow rate (mL/min)	30
	Air flow rate (mL/min)	300
	Initial temperature ($^{\circ}$ C)	80 (Holding time: 1min)
Oven setting	Ramping ($^{\circ}$ C/min)	5
	Final temperature ($^{\circ}$ C)	250 (Holding time: 3min)
	Total analysis time (min)	38

Table S2. Properties of the Raney Ni and Co catalysts

(a) Chemisorption composition (wt.%)

	Raney Ni	Raney Co
Ni	92.8	2.8
Co	0	91.3
Al	6.8	3.5
Fe	0.4	0.3
Cr	0	2.1

(b) chemisorption and physisorption data

Catalyst	H ₂ uptake (mmol g ⁻¹)	BET surface area (m ² g ⁻¹)	Total pore volume ^a (cm ³ g ⁻¹)	Average pore diameter (nm)
Raney Ni	0.173	18.4	0.029	4.8
Raney Co	0.065	25.8	0.034	5.3

Table S3. Detailed stream data associated with Figure 6 in the main text

Stream	1	2	3	4	5	6	7	8	9	10
Temperature [K]	298.15	409.90	350.15	353.26	298.15	733.74	353.15	352.88	353.15	354.13
Pressure [bar]	1	1	1	80	7	87	80	80	80	1
Enthalpy Flow [MW]	-6.56	-19.16	-22.68	-22.57	0.00	0.34	0.04	-22.53	-24.14	-24.14
Mass Flows [kt/y]										
ADN	20.50	20.50	20.50	20.50				20.50	0.20	0.20
HMDA	4.34	98.01	98.01	98.01				98.01	118.39	118.39
AZEPANE		0.02	0.02	0.02				0.02	0.23	0.23
H ₂					1.53	1.53	1.53	1.53	0.06	0.06
N H ₃									0.04	0.04
AHN		0.35	0.35	0.35				0.35	1.49	1.49
H ₂ O	10.39	15.37	15.37	15.37				15.37	15.37	15.37
NaOH	0.16	0.16	0.16	0.16				0.16	0.16	0.16
EtOH	4.94	49.39	49.39	49.39				49.39	49.39	49.39
Total flow	40.34	183.80	183.80	183.80	1.53	1.53	1.53	185.32	185.32	185.32
Stream	11	12	13	14	15	16	17	18	19	20
Temperature [K]	363.61	353.98	353.98	353.98	361.08	471.06	471.52	471.52	483.55	471.52
Pressure [bar]	1	1	1	1	1	1	1	1	1	1
Enthalpy Flow [MW]	-15.89	-10.18	0.00	-10.86	-6.77	-4.00	-2.17	-0.43	-0.07	-1.74
Mass Flows [kt/y]										
ADN					0.00	0.20	0.00	0.00	0.20	0.00
HMDA	0.12				0.12	118.27	117.09	23.42	1.18	93.67
AZEPANE	0.21				0.21	0.02	0.02	0.00	0.00	0.01
H ₂	0.06	0.06	0.06							
N H ₃	0.04	0.04	0.04							

AHN	0.05			0.05	1.44	0.43	0.09	1.01	0.35	
H ₂ O	15.31	4.93		4.93	10.38	0.06	0.06	0.01	0.00	0.05
NaOH						0.16			0.16	
EtOH	49.39	44.45		44.45	4.94					
Total flow	65.17	49.47	0.09	49.38	15.69	120.16	117.60	23.52	2.56	94.08

Table S4. Project cost worksheet including total direct cost and total capital investment for the integrated process strategy (R5_CNi)

Sub-processing steps			Installed costs (US\$)
Hydrogenation			5,604,694
Pump			279,800
Compressor			1,991,100
Reactor			3,293,200
HMDA purification			3,472,249
Distillation column 1			914,624
Distillation column 2			1,204,423
Distillation column 3			1,353,200
Utilities (Heat exchanger network)			1,657,229
Total installed cost			10,734,172
Site development	4.0%	of ISBL [#]	406,623
Land			4,200,000
Total direct cost (TDC)			15,340,79
Prorateable expenses	10.0%	of TDC(WO land)	1,114,079
Field expenses	10.0%	of TDC(WO land)	1,114,079
Home office & construction fee	20.0%	of TDC(WO land)	2,228,159
Project contingency	10.0%	of TDC(WO land)	1,114,079
Other costs (Start-Up, Permits, etc.)	10.0%	of TDC(WO land)	1,114,079
Total indirect cost			6,684,477
Fixed capital investment (FCI)			22,025,272
Land			4,200,000
Working capital	5.0%	of FCI	1,101,264
Total capital investment (TCI)			23,126,535
[#] Inside-battery-limits (ISBL) equipment costs include pretreatment, conversion and recovery steps.			
Fixed operating			5,933,535
Salaries			2,694,000
Benefits and general overhead			2,424,600
Maintenance	3.0%	of ISBL [#]	660,758
Insurance and taxes	0.7%	of FCI [*]	154,177
[#] Inside-battery-limits (ISBL) equipment costs include pretreatment, conversion and recovery steps.			
[*] Fixed capital investment			

Table S5. Discounted cash flow sheet (R5_CNi)

	-2	-1	0	1	2	3	4	5	6	7	8
Investment											
Fixed Capital Investment	704,809	5,286,065	2,819,235								
Land	4,200,000										
Working Capital			1,101,264								
Loan											
Loan Payment				1,969,449	1,969,449	1,969,449	1,969,449	1,969,449	1,969,449	1,969,449	1,969,449
Loan Interest Payment	84,577	718,905	1,057,213	1,057,213	984,234	905,417	820,294	728,362	629,075	521,845	406,037
Loan Principal	1,057,213	8,986,311	13,215,163	12,302,927	11,317,712	10,253,680	9,104,526	7,863,439	6,523,065	5,075,461	3,512,049
Annual sales											
HMDA sale				33,760,332	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237
Total Annual Sales				33,760,332	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237
Annual Manufacturing Costs											
Raw Materials and utility				27,033,593	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832
Fixed Operating Costs				5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535
Total Product Cost				32,967,128	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367
Annual Depreciation											
	7-Year MACRS schedule										
Total Plant MACRS Schedule				14%	24%	17%	12%	9%	9%	9%	4%
Depreciation				3,147,411	5,393,989	3,852,220	2,750,956	1,966,857	1,964,654	1,966,857	982,327
Net Revenue				-	-	-	242,619	1,118,651	1,220,140	1,325,168	2,425,506
Losses				-	-	-	-	-	-	-	-
Forward Taxable Income				3,411,420	2,564,353	943,767	6,919,540	6,676,921	5,558,271	4,338,130	3,012,962
Income				3,411,420	5,975,773	6,919,540	6,676,921	5,558,271	4,338,130	3,012,962	587,457

Income Tax				-	-	-	-	-	-	-	-
Annual Cash Income				-							
Discount Factor	1.21	1.10	1	1,176,244	1,844,421	1,844,421	1,844,421	1,844,421	1,844,421	1,844,421	1,844,421
Annual Present Value				0.91	0.83	0.75	0.68	0.62	0.56	0.51	0.47
Total Capital Investment + Interest	6,037,157	6,605,467	4,977,711	-	1,524,315	1,385,741	1,259,764	1,145,240	1,041,127	946,479	860,436
Net Present Worth											

Year	9	10	11	12	13	14	15	16	17	18	19
Investment											
Fixed Capital Investment											
Land											
Working Capital											
Loan											
Loan Payment	1,969,449	1,969,449									
Loan Interest Payment	280,964	145,885									
Loan Principal	1,823,564	0									
Annual sales											
HMDA sale	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237
Total Annual Sales	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237
Annual Manufacturing Costs											
Raw Materials	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832

and utility												
Fixed Operating Costs	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535
Total Product Cost	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367
Annual Depreciation												
Total Plant MACRS Schedule Depreciation												
Net Revenue	3,532,906	3,667,985	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870
Losses Forward Taxable Income	587,457	-	-	-	-	-	-	-	-	-	-	-
Income Tax	883,635	1,100,395	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161
Annual Cash Income	960,786	744,025	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709
Discount Factor	0.42	0.39	0.35	0.32	0.29	0.26	0.24	0.22	0.20	0.18	0.16	
Annual Present Value	407,467	286,854	935,717	850,651	773,320	703,018	639,107	581,006	528,188	480,171	436,519	
Total Capital Investment + Interest Net Present Worth												

Year	20	21	22	23	24	25	26	27	28	29	30
Investment											
Fixed Capital Investment											
Land											

Working Capital												-
												5,301,264
Loan												
Loan Payment												
Loan Interest Payment												
Loan Principal												
Annual sales												
HMDA sale	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237
Total Annual Sales	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237	38,583,237
Annual Manufacturing Costs												
Raw Materials and utility	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832	28,835,832
Fixed Operating Costs	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535	5,933,535
Total Product Cost	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367	34,769,367
Annual Depreciation												
Total Plant MACRS Schedule Depreciation												
Net Revenue	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870
Losses Forward	-	-	-	-	-	-	-	-	-	-	-	-
Taxable Income	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870	3,813,870
Income Tax	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161	1,144,161
Annual Cash	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709	2,669,709

Income											
Discount	0.15	0.14	0.12	0.11	0.10	0.09	0.08	0.08	0.07	0.06	0.06
Factor											
Annual											
Present	396,835	360,759	327,963	298,148	271,044	246,403	224,003	203,639	185,127	168,297	152,997
Value											
Total											
Capital											
Investment											
+ Interest											
Net Present											
Worth											