

Supplementary data

Energy intensity and environmental impact metrics of the back-end separation of ethylene plant by thermodynamic analysis

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Table S1

Columns modified case summary: N: number of total stages; NF1, NF2, NF3 are the feed stages; RR is the reflux ratio; F is the total mass flow rate; P is the column pressure; TF1, TF2, TF3 are the feed temperatures, and PF1, PF2, PF3 are the feed Pressures.

Operation	Column 1		Column 2		Column 3	
	Base	Modified	Base	Modified	Base	Modified
N	50	55	50	55	60	66
NF	NF1=25	NF1=25	28	33	35	35
	NF2=15	NF2=15				
	NF3=10	NF3=11				
Mole RR	0.65	0.33	0.54	0.53	4.75	4.49
F (mt/hr)	F1=97.3	F1=97.3	175.86	175.86	173.23	173.23
	F2=59.82	F2=59.82				
	F3=3.74	F3=3.74				
P (bar)	35.15	35.15	23.9	23.9	16.87	16.87
TF (°C)	TF1= -37	TF1= -30	5	9	-24.6	-24.6
	TF2= -98	TF2= -98				
	TF3= -129	TF3= -129				
PF (bar)	PF1=37.3	PF1=37.30	35.15	35.15	17.6	17.6
	PF2=37	PF2=37				
	PF3=37	PF3=37				
Condenser duty (MW)	-0.29	-0.55	-6.38	-8.22	-37.81	-40.30
Condenser temp.(°C)	-99.58	-99.54	-13.68	-13.68	-35.92	-35.92
Reflux rate (mt/hr)	2.21	1.91	74.24	75.03	391.44	373.84
Distillate rate (mt/hr)	2.99	2.99	137.23	137.23	80.41	80.41
			1			
Reboiler duty (MW)	9.33	9.68	16.26	18.09	32.2	34.34
Reboiler temp.(°C)	5.53	5.53	74.41	74.41	-15	-14.93
Boilup rate (mt/hr)	138.75	128.10	204.07	204.92	329.2	308.33
Bottoms rate (mt/hr)	157.86	157.86	20.63	20.63	56.82	56.82

Table S2

Sustainability indicators for column 1 with modifications: N=50→55; NF1=25, NF2=15, NF3=11; RR=0.65→0.328; TF1= -37 °C →-30 °C.

Material intensity indicators	Column 1		
	Base Case	Modified Case	Change %
Feed 1 rate (mt/day)	2335.22	2335.22	0
Feed 2 rate (mt/day)	1435.73	1435.73	0
Feed 3 rate (mt/day)	89.66	89.66	0
Distillate rate (mt/day)	71.96	71.96	0
Bottoms rate(mt/day)	3788.66	3788.66	0
Energy intensity indicators			
Condenser duty, kW	-296.23	-286.83	-3.17
Reboiler duty, kW	9327.48	8769.74	-5.98
Feed conditioning duty, kW	0	548.28	-
Utility cost in condenser, \$/day	1083.41	1049.04	-3.17
Utility cost in reboiler, \$/day	2555.49	2402.68	-5.98
Utility cost in feed conditioning, \$/day	0	89.76	+100
Total exergy loss, kW	1585.00	124.34	-92.15
Environmental impact indicators			
Condenser CO ₂ emission ¹ , mt /day	1.43	1.38	-3.50
Reboiler CO ₂ emission ¹ , mt /day	45.04	42.35	-5.97
Feed conditioning CO ₂ emission ¹ , mt /day	0	2.64	-

¹Emission based on US-EPA-Rule-E9-5711 and natural gas.

Table S3

Sustainability indicators for column 2 with the modifications: N=50→55; NF=33; RR=0.65→0.53;

TF= 5 °C → 9 °C.

Material intensity indicators	Column 2		
	Base Case	Modified Case	Change %
Feed rate (mt/day)	3,788.66	3,788.66	0
Distillate rate (mt/day)	3,293.55	3293.55	0
Bottoms rate(mt/day)	495.10	495.10	0
Energy intensity indicators			
Condenser duty, kW	-6,384.75	-6,839.19	+6.64
Reboiler duty, kW	16,260.30	11,123.40	-31.60
Feed conditioning duty, kW	0	5591.27	-
Utility cost in condenser, \$/day	6,498.34	6,960.87	+6.64
Utility cost in reboiler, \$/day	2,663.15	1,821.82	-31.60
Utility cost in feed conditioning, \$/day	0	915.60	-
Total exergy loss, kW	3,726.13	2,343.95	-37.10
Environmental impact indicators			
Condenser CO ₂ emission ¹ , mt /day	30.83	33.02	+6.63
Reboiler CO ₂ emission ¹ , mt /day	78.52	53.71	-31.60
Feed conditioning CO ₂ emission ¹ , mt /day	0	26.88	-

¹Emission based on US-EPA-Rule-E9-5711, natural gas.**Table S4**

Sustainability indicators of column 3 with modifications: N=66; NF=35; RR=4.49.

Material intensity indicators	Column 3		
	Base Case	Modified Case	Change %
Feed rate (mt/day)	3,293.62	3,293.62	0
Distillate rate (mt/day)	1,929.82	1,929.82	0
Bottoms rate (mt/day)	1,363.80	1,363.80	0
Energy intensity indicators			
Condenser duty, kW	-37,814.20	-35,080.10	-7.23
Reboiler duty, kW	32,198.80	29,125.50	-9.54
Utility cost in condenser, \$/day	55,312.80	51,313.50	-7.23
Utility cost in reboiler, \$/day	8,821.66	7,979.65	-9.54
Total exergy loss, kW	1,681.69	1,389.02	-17.40
Environmental impact indicators			
Total condenser CO ₂ emission ¹ , mt /day	182.60	169.39	-7.23
Total reboiler CO ₂ emission ¹ , mt /day	155.48	140.64	-9.54

¹Emission based on US-EPA-Rule-E9-5711 and natural gas.

NQ curve analysis:

Column1:

Table S5 show four different cases of NQ curves analysis, each case gave different number of total stages, feed stage, duties, and reflux ratio. Table S5 is based on feed 2 (DEC1-F2) optimization with an objective function of minimizing the duties so case number 1 is the objective case.

Table S5

Column1 NQ curves result summary (AspenTech, 2013).

Case No.	Feed Stage	Total stages	Condenser duty, MW	Reboiler duty, MW	Reflux ratio, mole
→ 1	15	55	-0.272	9.303	0.382
2	12	53	-0.276	9.308	0.387
3	12	51	-0.280	9.311	0.393
4	14	49	-0.296	9.326	0.418

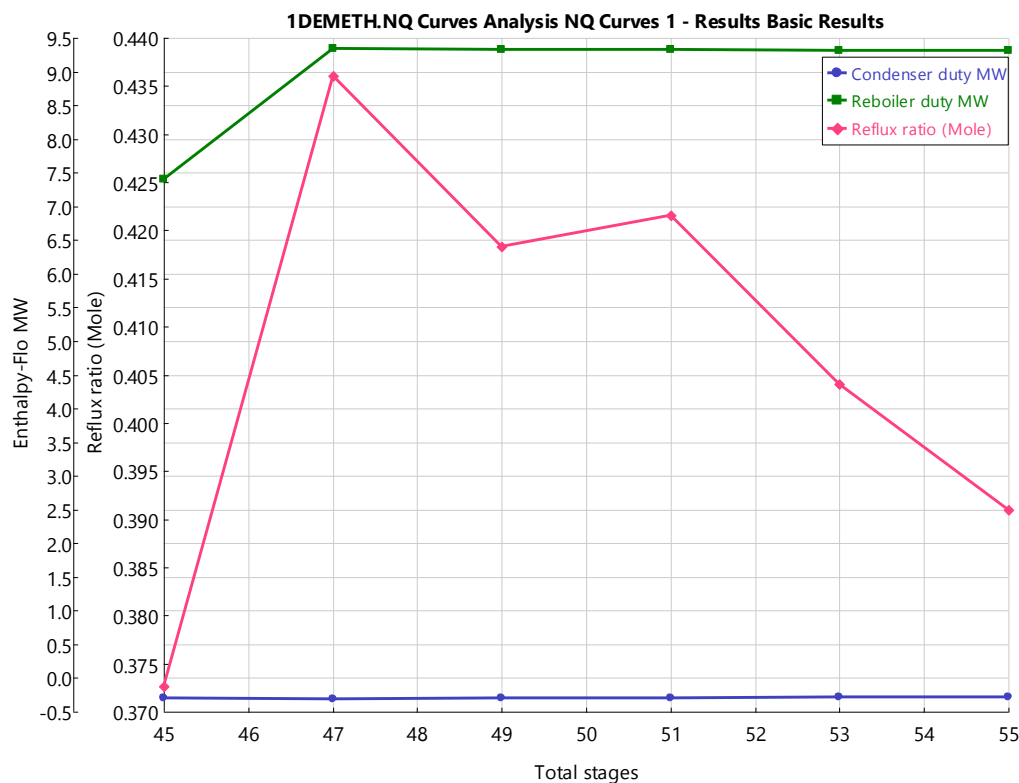


Fig. S1. Column 1 NQ curve curves results.

Column 2:

Table S6 show four different cases of NQ curves analysis, each case gave different number of total stages, feed stage, duties, and reflux ratio. Table S6 is based on bottom feed of column 1 (1BOT) optimization with an objective function of minimizing the duties so case number 1 is the objective case.

Table S6

Column 2 NQ curves result summary (AspenTech, 2013).

Case No.	Feed stage	Total stages	Condenser duty, MW	Reboiler duty, MW	Reflux ratio, mole
→ 1	33	55	-6.316	16.192	0.531
2	31	53	-6.338	16.214	0.533
3	30	51	-6.366	16.242	0.535
4	28	49	-6.399	16.275	0.538
5	26	47	-6.442	16.317	0.542

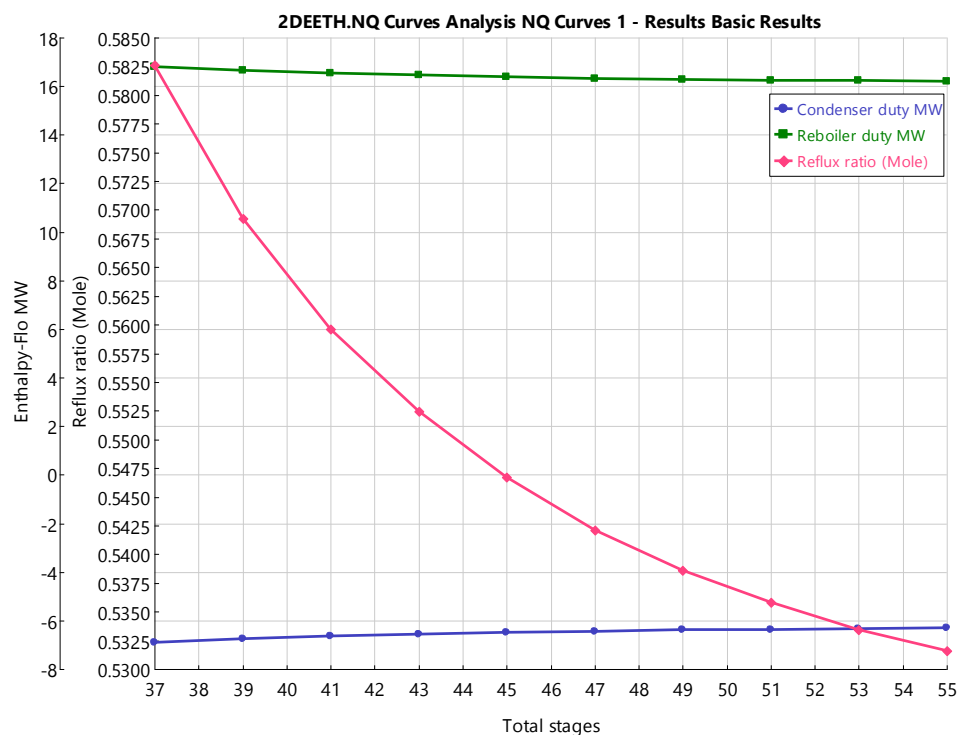


Fig. S2. Column 2 NQ curve curves results.

Column 3:

Table S7 shows three different cases of NQ curves analysis, each case gave different number of total stages, feed stage, duties, and reflux ratio. Table S7 is based on feed 3 (C2FRAC-1) optimization with an objective function of minimizing the duties so case number 1 is the objective case.

Table S7

Column 3 NQ curves result summary (Aspen Technology, 2013).

Case No.	Feed stage	Total stages	Condenser duty, MW	Reboiler duty, MW	Reflux ratio, mole
→ 1	35	66	-34.911	29.296	4.494
2	35	64	-35.553	29.937	4.576
3	34	62	-36.361	30.746	4.681

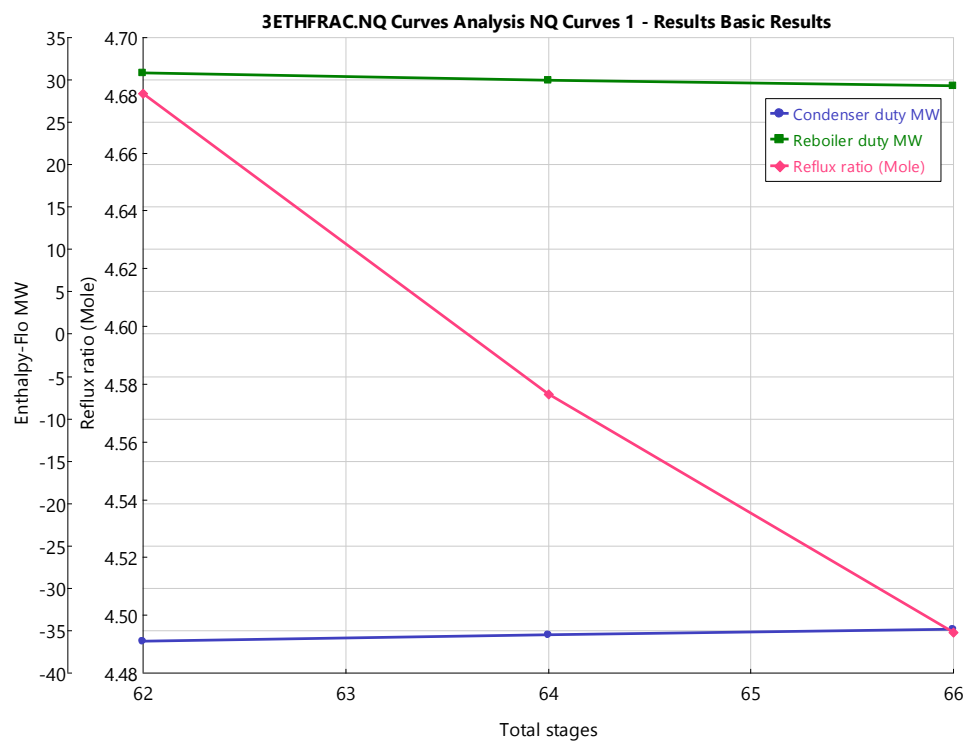


Fig. S3. Column 3 NQ curve curves results.

Utility Price:

Table S8

Utilities energy price

Utility	T _{in} (°C)	T _{out} (°C)	Energy Price (\$/kJ)
Refrigerant 1	-65	-64	2.48E ⁻⁵
Refrigerant 2	-102	-101	4.23E ⁻⁵
Refrigerant 3	-6.66	-6.72	3.17E ⁻⁶
Refrigerant 5	-18	-17	1.17E ⁻⁵
Refrigerant 6	-40.03	-40	1.69E ⁻⁵
LPS	125	124	1.89E ⁻⁵
CW	20	25	2.12E ⁻⁷

Balance summary:

Table S9

Columns mass, mole, and energy balance.

Column 1	Base Case			Modified Case		
	In	Out	Relative difference	In	Out	Relative difference
Mole, kmole/hr	5443.1300	5443.1300	0.0000	5443.1300	5443.1300	0.0000
Mass, tonne/hr	160.8590	160.8590	0.0000	160.8590	160.8590	0.0000
Enthalpy, MW	-30.1715	-21.1402	-0.2993	-29.6232	-21.1403	-0.2863
Column 2						
Mole, kmole/hr	5172.0600	5172.0600	0.0000	5172.0700	5172.0700	0.0000
Mass, tonne/hr	157.8610	157.8610	0.0000	157.8610	157.8610	0.0000
Enthalpy, MW	-17.5982	-7.7226	-0.5612	-12.0070	-7.7227	-0.3568
Column3						
Mole, kmole/hr	4754.3100	4754.3100	0.0000	4754.3100	4754.3100	0.0000
Mass, tonne/hr	137.2340	137.2340	0.0000	137.2340	137.2340	0.0000
Enthalpy, MW	-6.7004	-12.3157	0.4559	-6.3607	-12.3153	0.4835

Table S10:Columns CO₂ emissions summary.

Column 1	Base case emissions	Modified case emissions
Feed streams CO ₂ , tonne/hr	53.8820	53.8819
Product streams CO ₂ , tonne/hr	53.8820	53.8819
Net streams CO ₂ production, tonne/hr	0.0000	0.0000
Utilities CO ₂ production, tonne/hr	1.9363	1.8222
Total	1.9363	1.8222
Column2		
Feed streams CO ₂ , tonne/hr	0.0871	0.0871
Product streams CO ₂ , tonne/hr	0.0871	0.0871
Net streams CO ₂ production, tonne/hr	0.0000	0.0000
Utilities CO ₂ production, tonne/hr	4.5562	3.6141
Total	4.5562	3.6141
Column 3		
Feed streams CO ₂ , tonne/hr	0.0871	0.0871
Product streams CO ₂ , tonne/hr	0.0871	0.0871
Net streams CO ₂ production, tonne/hr	0.0000	0.0000
Utilites CO ₂ production, tonne/hr	14.0869	12.9184
Total	14.0869	12.9184

*Stream results summary:***Table S11**

Column1 stream results summary

Column 1	Feed 1	Feed 2	Feed 3	Distillate	Bottoms
Phase:	Mixed	Liquid	Liquid	Vapor	Liquid
Mole flow, kmol/hr					
ethane	1185.5370	670.9029	25.2248	0.0120	1881.6520
ethylene	1483.6250	1294.2670	97.0556	8.1317	2866.8160
hydrogen	64.8051	36.5320	1.8988	103.2360	0.0000
methane	50.1724	94.5175	15.2456	159.6769	0.2586
acetylen	0.5034	0.3351	0.0163	0.0003	0.8544
propylen	193.0465	29.1565	0.1162	0.0000	222.3192
propane	76.1076	9.0117	0.0239	0.0000	85.1432
butadien	27.4539	0.8076	0.0002	0.0000	28.2617
butene	13.4285	0.4196	0.0001	0.0000	13.8482
butane	13.4457	0.6843	0.0008	0.0000	14.1309

benzene	58.6671	0.1172	0.0000	0.0000	58.7844
water	0.0000	0.0000	0.0000	0.0000	0.0000
Mole fraction					
ethane	0.3744	0.3140	0.1807	0.0000	0.3638
ethylene	0.4685	0.6057	0.6953	0.0300	0.5543
hydrogen	0.0205	0.0171	0.0136	0.3809	0.0000
methane	0.0158	0.0442	0.1092	0.5891	0.0001
acetylene	0.0002	0.0002	0.0001	0.0000	0.0002
propylene	0.0610	0.0136	0.0008	0.0000	0.0430
propane	0.0240	0.0042	0.0002	0.0000	0.0165
butadiene	0.0087	0.0004	0.0000	0.0000	0.0055
butene	0.0042	0.0002	0.0000	0.0000	0.0027
butane	0.0042	0.0003	0.0000	0.0000	0.0027
benzene	0.0185	0.0001	0.0000	0.0000	0.0114
water	0.0000	0.0000	0.0000	0.0000	0.0000
Mole flow, kmol/hr	3166.7920	2136.7520	139.5824	271.0569	5172.0690
Temperature, °C	-30.0000	-98.3333	-128.8889	-99.5942	5.4838
Pressure, kg/sqcm	37.6142	37.2627	37.2627	35.1535	35.1535
Vapor fraction	0.0013	0.0000	0.0000	1.0000	0.0000
Liquid fraction	0.9987	1.0000	1.0000	0.0000	1.0000
Solid fraction	0.0000	0.0000	0.0000	0.0000	0.0000
Molar enthalpy, kJ/kmol	22279.2300	-16478.0500	6307.1190	-47042.3400	12249.2400
Molar entropy, kJ/kmol-k	-183.0842	-187.5316	-182.0669	-92.12668	-165.3717
Molar density, kmol/m ³	15.1632	19.9400	21.9583	2.8073	11.6569
Average molecular weight	30.7254	27.9967	26.7664	11.0614	30.5218
Carbon equivalents - US EPA (2009), tonne/hr	16.9030	31.8428	5.1362	53.7948	0.0871
Exergy flow rate, MW	7.9344	6.9959	0.5339	0.7577	12.2128

Table S12:

Column 2 stream results summary.

Column 2	Feed	Distillate	Bottoms
Phase:	Mixed	Vapor	Liquid
Mole flow, kmol/hr			
ethane	1881.6520	1881.6310	0.0209
ethylene	2866.8160	2866.8160	0.0001
methane	0.2586	0.2586	0.0000
acetylene	0.8544	0.8544	0.0000
propylene	222.3192	4.7454	217.5737
propane	85.1432	0.0089	85.1343
butadiene	28.2617	0.0000	28.2617

butene	13.8482	0.0000	13.8482
butane	14.1309	0.0000	14.1309
benzene	58.7844	0.0000	58.7844
Mole fraction			
ethane	0.3638	0.3958	0.0001
ethylene	0.5543	0.6030	0.0000
methane	0.0001	0.0001	0.0000
acetylene	0.0002	0.0002	0.0000
propylene	0.0430	0.0010	0.5208
propane	0.0165	0.0000	0.2038
butadiene	0.0055	0.0000	0.0677
butene	0.0027	0.0000	0.0331
butane	0.0027	0.0000	0.0338
benzene	0.0114	0.0000	0.1407
Mole flow, kmol/hr	5172.0690	4754.3150	417.7542
Temperature, °C	9.0000	-13.6888	74.4075
Pressure, kg/sqcm	35.1535	23.9044	23.9044
Vapor fraction	0.5300	1.0000	0.0000
Liquid fraction	0.4700	0.0000	1.0000
Molar enthalpy, kJ/kmol	-8357.4550	-5073.3520	-8813.0480
Molar entropy, kJ/kmol-k	-151.4820	-133.0952	-226.9428
Molar density, kmol/m ³	3.7418	1.5360	9.7867
Average molecular weight	30.5218	28.8646	49.3815
Carbon equivalents - US EPA (2009), tonne/hr	0.0871	0.0871	0.0000
Exergy flow rate, MW	11.8544	10.0100	0.5178

Table S13:
Column 3 stream results summary.

Column 3	Feed	Distillate	Bottoms
Phase:	Vapor	Vapor	Liquid
Mole flow, kmol/hr			
ethane	1882.1380	2.5361	1879.6020
ethylene	2867.1640	2863.3880	3.7763
hydrogen	0.0000	0.0000	0.0000
methane	0.2586	0.2586	0.0000
acetylene	0.0000	0.0000	0.0000
propylene	4.7454	0.0000	4.7454
propane	0.0089	0.0000	0.0089
Mole fraction			
ethane	0.3959	0.0009	0.9955
ethylene	0.6031	0.9990	0.0020

methane	0.0001	0.0001	0.0000
propylene	0.0010	0.0000	0.0025
Mole flow, kmol/hr	4754.3150	2866.1830	1888.1320
Temperature, °C	-20.0000	-35.9207	-14.9333
Pressure, kg/sqcm	17.5767	16.8737	16.8737
Vapor fraction	1.0000	1.0000	0.0000
Liquid fraction	0.0000	0.0000	1.0000
Molar enthalpy, kJ/kmol	-4816.3710	48643.2900	-97321.3800
Molar entropy, kJ/moll-k	-0.1300	-0.0895	-0.2487
Molar density, kmol/m ³	1.0422	1.0849	13.6791
Average molecular weight	28.8652	28.0545	30.0959
Carbon equivalents - US EPA (2009), tonne/hr	0.0871	0.0871	0.0000
Exergy flow rate, MW	9.1910	5.6118	4.4228