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

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ORIGINAL RESEARCH

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

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Abstract This study presents metrics of energy intensity and environmental impact of the back-end separation of ethylene plant consisting three interacting distillation columns by thermodynamic analysis. The objective is to explore the scope of reducing the energy for utilities and CO_2 emissions. Thermodynamic analysis is carried out using the column targeting tool (CTT) to address the sustainability metrics of 'Energy Intensity.' CTT is based on the 'Practical Near-Minimum Thermodynamic Condition' representing a close to practical reversible column operation. Environmental impact metrics are estimated from the carbon tracking options. The carbon tracking are estimated by the CO_2 emission data source of US-EPA-Rule-E9-5711 using natural gas as the primary fuel. The results show that the total reductions in exergy loss and the total hot and cold utility are around 44 and 10 %, respectively; the total reductions in carbon dioxide are around 14 %. These improvements lead to considerable reductions in the operating costs. Thermodynamic analysis helps estimating and improving the energy and environmental sustainability metrics and hence can lead to a more sustainable separation by distillation columns.

Keywords Ethylene plant · Distillation column · Column targeting tool · Exergy loss profiles · Energy intensity · Environmental impact metrics

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Introduction

Distillation-based separations consume about 40 % of the total energy used in petrochemical and chemical process industries in North America [1, 2]. The relatively high purity recovery and low relative volatility require toll distillation columns with very high installation and operating costs in ethylene plants [3]. Therefore, the olefin/paraffin separation process of ethylene, propylene and other high-volume olefin petrochemicals is highly energy-intensive, and hence impacts environment. Cryogenic distillation is the commercially viable separation; however, it consumes over 20 Gigajoules of energy for every ton of ethylene produced. This energy consumption is associated with significant greenhouse gas emission and depletion of non-renewable energy resources. Consequently, there is a strong economic incentive to reduce the costs through improved process designs for the back-end separation of ethylene by distillation [3, 4].

A typical distillation column resembles a heat engine [2] delivering separation work by using heat at a high temperature in the reboiler and discharging most of it to the environment at a lower temperature in the condenser [5, 6]. One of the thermodynamic methodologies to assess the distillation column operation is the column targeting tool (CTT), which is based on the practical near-minimum thermodynamic condition (PNMTC) approximation representing a practical and close to reversible operation [7, 8]. CTT exploits the capabilities for thermal and hydraulic analyses of distillation columns [4, 7] to identify the targets for possible column retrofits for (1) feed stage location, (2) reflux ratio, (3) feed conditioning, and (4) side condensing and/or reboiling to reduce the cost of utilities and improve the overall energy efficiency [9–11]. The 'carbon tracking' options of the Aspen Plus can help quantify the reduction in CO_2 emission in a simulation environment [8].

Sustainability has environmental, economic, and social dimensions [12, 13] and requires the responsible use of energy resources and reduction in CO_2 emission. The three intersecting dimensions illustrate the 3D-sustainability metrics that include nonrenewable energy use, toxic, and pollutant emissions per unit product [14, 15]. If nonrenewable, energy usage affects environment adversely through the emission of pollutants such as CO_2. Therefore, a comparative assessment with the sustainability metrics may prove useful in identifying the scope for retrofits for possible reductions of the waste energy and emission of CO_2 for the three interacting distillation columns of a typical ethylene plant. The energy metrics are estimated from the CTT, while the carbon emission from the data source of US-EPA-Rule-E9-5711 using the fuel source of natural gas.

Ethylene plant

Ethylene is produced by steam cracking in which light hydrocarbons are heated to 750–950 °C, inducing numerous reactions. Ethylene is separated from the resulting complex mixture by repeated compression and distillation processes. The separation of ethylene from ethane by distillation is normally the final step in the production of ethylene. The separation of ethylene is expensive because (1) the required purity of ethylene usually exceeds 99.9 % and (2) the relative volatility of ethylene to ethane is moderately small ranging from about 1.13 for high-pressure mixtures rich in ethylene to 2.34 for low-pressure mixtures rich in ethane. Ethylene fractionation separates ethylene as a highly pure overhead product, 99.9 wt%, free of olefins, acetylenes, dienes, and water. Ethylene production is close to the historic mid-range of 145 million lb/day in the U. S. States. Global production of ethylene was about 141 million mt in 2011 [3]. Approximately 90 % of ethylene is used to produce ethylene oxide, ethylene dichloride, ethyl benzene, and polyethylene.

Figure 1 shows the back-end separation of a conventional ethylene plant. As shown in Fig. 1, stream 12 has a flow of 20.39 kg/s, at 16 °C and 39 bar, consists of 5.83 kg/s of ethane, 10.98 kg/s of ethylene, 1.96 kg/s of hydrogen, 1.12 kg/s of methane, 0.003 kg/s of acetylene, 0.342 kg/s of propylene, 0.111 kg/s of propane, 0.012 kg/s of butadiene, 0.007 kg/s of butene, 0.011 kg/s of butane, and 0.003 kg/s of benzene. The feed enters a splitter S2. The separated streams pass through reactors and flash separators till they reach the separation section containing the three RadFrac columns. The streams pass through the columns to produce ethylene as the distillate from column 3 and ethane as the bottom product which is recycled to C2REC reactor. Propylene is the bottom stream of column 2. The reactor between column 2 and column 3 converts the small amount of acetylene (0.022 ton/h) to ethylene, which is converted into ethane completely using 1.36 kmol hydrogen at −37.78 °C and 21.1 bar. The reactor receives the 137.23 ton/h gas distillate at −13.7 °C and 23.9 bar from column 2. The outlet of the reactor is 137.23 ton/h consisting of 41.2 wt% of ethane and 58.6 wt% of ethylene.

This study focuses on the separation section having three distillation columns as shown in Fig. 1. Column 1 has three feeds and the overhead contains the hydrogen and methane which are recycled, while the bottom flow contains the mixture of ethane, ethylene, propylene, butadiene, butane, butane, and benzene which are separated in column 2 to a bottom flow containing propylene, propane, butadiene, butane, and benzene. Ethane and ethylene in the

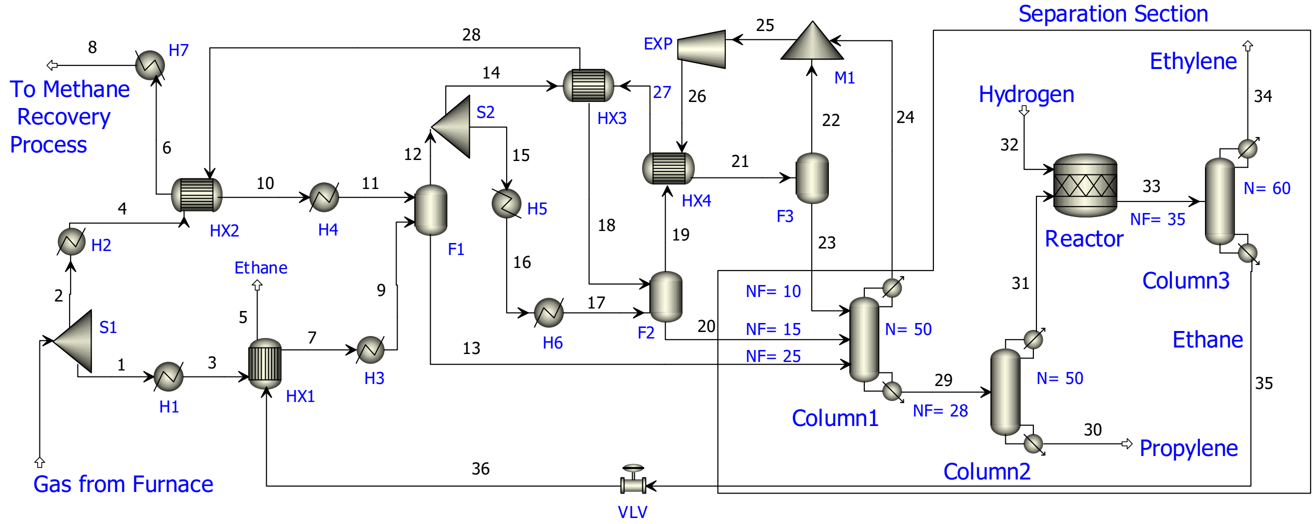


Fig. 1 Process flow diagram of ethylene plant with back-end separation

Table 1 Column base case configurations: *N* number of total stages; *NF1*, *NF2*, and *NF*3 are the feed stages; *RR* is the molar reflux ratio; *F* is the total mass flow rate; *P* is the column pressure; *TF1*, *TF2*, and *TF3* are the feed temperatures, and *PF1*, *PF2*, and *PF3* are the feed pressures [8]

Configuration	Column 1	Column 2	Column 3
N	50	50	60
NF	$NF1 = 25$	28	35
	$NF2 = 15$		
	$NF3 = 10$		
Mole RR	0.65	0.53	4.75
F (kg/s)	$F1 = 27.03$	43.85	38.12
	$F2 = 16.62$		
	$F3 = 1.04$		
P (kPa)	3447.38	2344.22	1654.74
TF (°C)	$TF1 = -37$	5.50	−24.60
	$TF2 = -98$		
	$TF3 = -129$		
PF (kPa)	$PF1 = 3688.71$	3447.38	1723.69
	$PF2 = 3447.38$		
	$PF3 = 3447.38$		
Condenser duty (MW)	−0.29	−6.38	−37.81
Condenser temp. (°C)	−99.58	−13.68	−35.92
Reflux rate (kg/s)	0.59	22.09	100.87
Distillate rate (kg/s)	0.83	38.12	22.33
Reboiler duty (MW)	9.33	16.26	32.20
Reboiler temp. (°C)	5.53	74.41	−15.00
Boilup rate (kg/s)	36.23	6.76	82.71
Bottoms rate (kg/s)	43.85	5.73	15.78

presence of hydrogen go to the overhead and finally become the feed to column 3 where ethylene is the overhead product, while the ethane in the bottom is recycled. Table 1 shows the base configurations of the three columns. The Soave–Redlich–Kwong equation of state is used in the simulation of the plant.

Materials and methods

Sustainability

The Center for Waste Reduction Technologies (CWRT) of the American Institute of Chemical Engineers (AIChE) and the Institution of Chemical Engineers (IChemE) proposed a set of sustainability metrics applicable to a specific process [12–15, 22, 23]:

- Material intensity (nonrenewable resources of raw materials, solvents/unit mass of product(s))
- Energy intensity (nonrenewable energy/unit mass of product(s))
- Potential environmental impact (pollutants and emissions/unit mass of product(s))
- Potential chemical risk (toxic emissions/unit mass of product(s))

Carbon tracking

The carbon tracking option may be based on the CO_2 emission factor data source of US-EPA-Rule-E9-5711 (used in this study) or EU-2007/589/EC as well as on a selected fuel source, such as natural gas, biogas, petroleum, or coal as summarized in Table 2.

For distillation column operations, this study uses a comparative assessment with the following sustainability metrics:

- 'Energy intensity' as nonrenewable energy/unit mass of product(s) by using the CTT.
- 'Potential environmental impact' as emissions and cost/unit mass of product(s) by using the 'carbon tracking' options.

Column targeting tool

The column targeting tool is a retrofit tool for lowering cost of operation through modified operating conditions and providing insight into understanding tray/packing capacity limitations. The CTT is based on the practical near-minimum thermodynamic condition representing a close to practical reversible column operation [20]. The CTT

Table 2 Carbon dioxide emission rates for various CO_2 emission factor data sources and fuel sources [8]

Fuel sources	CO_2 emission factor data sources, lb/MMBtu	
	US-EPA-Rule-E9-5711	EU-2007/589/EC
Natural gas	130.00	130.49
Petroleum-coke	250.21	226.78
Coal bituminous	229.02	219.81
Coal anthracite	253.88	228.41
Crude oil	182.66	170.49
Bio gas	127.67	0

performs (1) thermal, (2) exergy, and (3) hydraulic analyses capabilities that can help identify the targets for appropriate column modifications in order to (1) reduce utilities cost, (2) improve energy efficiency, (3) reduce capital cost by improving thermodynamic driving forces, and (4) facilitate column debottlenecking [4, 10–17, 19, 21]. These capabilities within the CTT are summarized below.

Thermal analysis

Thermal analysis capability distributes reboiling and condensing loads over the temperature range of operation to help identify design targets for improvements in energy consumption and efficiency [1, 2, 5]. In order to achieve this, the thermal analysis produces 'Column Grand Composite Curves' (CGCC) and 'Exergy Loss Profiles.' The user makes changes to column configurations and specifications until CGCCs and exergy profiles display closer actual and ideal operations [14, 16]. The CGCCs are displayed as the stage-enthalpy (Stage-*H*) or temperature–enthalpy (*T*–*H*). They represent the theoretical minimum heating and cooling requirements in the temperature range of separation. This approximation takes into account the inefficiencies introduced through column design and operation, such as mixing, pressure drops, multiple side-products, and side strippers. Using CGCC is significant because (1) it is a graphical tool to assess the current energy use and flow conditions of distillation operations, (2) it is based on the complex and rigorous stage-by-stage calculations, and (3) it can lead to the qualitative and quantitative guidance [4, 13, 15, 16] in identifying the targets for potential column modifications for the following:

1. Feed stage location (appropriate placement),
2. Reflux ratio modification (reflux ratio versus number of stages),
3. Feed conditioning (heating or cooling),
4. Side condensing or reboiling (adding side heater and/or cooler).

For estimation the enthalpy deficits, the equations for equilibrium and operating lines are solved simultaneously at each stage for specified light key and heavy key components. Using the equilibrium compositions of light *L* and heavy *H* key components, the enthalpies for the minimum vapor and liquid flows are obtained and used in the enthalpy balances at each stage to determine the net enthalpy deficits [10, 12, 19].

$$H_{\mathrm{def}} = H_{\mathrm{Lmin}} - H_{\mathrm{Vmin}} + H_D \quad \text{(before the feed stage)} \tag{1}$$

$$H_{\mathrm{def}} = H_{\mathrm{Lmin}} - H_{\mathrm{Vmin}} + H_D - H_{\mathrm{feed}} \quad \text{(after the feed stage)} \tag{2}$$

After adding the individual stage enthalpy deficits to the condenser duty, the enthalpy values are cascaded and plotted in the CGCC. This is called the top-down calculation procedure [10]. At the feed stage, mass and energy balances differ from an internal stage and the enthalpy deficit becomes

$$\begin{aligned} H_{\mathrm{def,F}} = Q_C + D[H_D + H_L(x_D - y_F^*)/(y_F^* - x_F^*) \\ - H_V(x_D - x_F^*)/(y_F^* - x_F^*)] \end{aligned} \tag{3}$$

The values of y_F^* and x_F^* may be obtained from an adiabatic flash for a single-phase feed, or from the constant relative volatility estimated with the converged compositions at the feed stage and feed quality. This procedure can be reformulated for multiple feeds and side products as well as different choices of the key components. In a CGCC, a pinch point near the feed stage occurs for nearly binary ideal mixtures. However, for nonideal multicomponent systems multiple pinches may exist in rectifying and stripping sections.

Exergy analysis

Physical exergy (Ex) is the maximum amount of work that may be performed theoretically by bringing a resource into equilibrium with its surrounding through a reversible process:

$$\mathrm{Ex} = \Delta H - T_o \Delta S, \tag{4}$$

where *H* and *S* are the enthalpy and entropy, respectively, and T_o is the reference temperature, which is usually assumed as the environmental temperature of 298.15 K. Exergy balance for a steady state system is

$$\begin{aligned} \sum_{\substack{\text{into}\\ \text{system}}} \left[\dot{n}\mathrm{Ex} + \dot{Q}\left(1 - \frac{T_o}{T_s}\right) + \dot{W}_s\right] \\ - \sum_{\substack{\text{out of}\\ \text{system}}} \left[\dot{n}\mathrm{Ex} + \dot{Q}\left(1 - \frac{T_o}{T_s}\right) + \dot{W}_s\right] = \dot{\mathrm{E}}\mathrm{x}_{\mathrm{loss}}, \end{aligned} \tag{5}$$

where $\dot{W}_s$ is the shaft work. In general, the exergy loss profiles can be used to examine the degradation of accessible work due to (1) momentum loss (pressure driving force), (2) thermal loss (temperature driving force), and (3) chemical potential loss (mass transfer driving force) [1, 8, 17, 20].

The exergy profiles are plotted as state-exergy loss or temperature-exergy loss. A part of accessible work potential is always lost in any real process. Exergy losses (destructions) represent inefficient use of available energy due to irreversibility and should be reduced by suitable modifications [12, 16]. As the exergy loss increases, the net heat duty has to increase to enable the column to achieve its required separation task. Consequently, smaller exergy loss means less waste energy.

Thermodynamic efficiency

Thermal efficiency can be defined as a thermal performance of an operation or a process. Thermodynamic efficiency is estimated depending on the sign of the main goal: Eq. (6) for the negative main goal and Eq. (7) for the positive one

$$\eta_{(-)\mathrm{Ex}_{\min}} = \frac{\mathrm{Ex}_{\min}}{\mathrm{Ex}_{\min} - \mathrm{Ex}_{\mathrm{loss}}} \tag{6}$$

$$\eta_{(+)\mathrm{Ex}_{\min}} = \frac{\mathrm{Ex}_{\min}}{\mathrm{Ex}_{\min} + \mathrm{Ex}_{\mathrm{loss}}} \tag{7}$$

The main goal is the minimum exergy loss in accomplishing that goal [24]. Minimum exergy determined by calculating the difference between exergies of products and the feed streams

$$\mathrm{Ex}_{\min} = \sum_{\mathrm{out}} \dot{n}\mathrm{Ex} - \sum_{\mathrm{in}} \dot{n}\mathrm{Ex}, \tag{8}$$

where $\dot{n}$ is the molar flow rate.

Hydraulic analysis

The hydraulics analysis produces the stage profiles for (1) thermodynamic ideal minimum flow, (2) hydraulic maximum flow, and (3) actual flow that help understand how the vapor and liquid flow rates in a column compare with the minimum (corresponding to the PNMTC) and maximum (corresponding to flooding) limits. Therefore, it can be used to identify and eliminate column bottlenecks [9–11]. Tray or packing rating for the entire column is necessary to activate the hydraulic analysis. In addition, allowable flooding factors (as fraction of total flooding) for flooding limit calculations can be specified. Hydraulic analysis helps identify the allowable limit for vapor flooding on the Tray Rating|Design/Pdrop or Pack Rating|Design/Pdrop options. The default values are 85 % for the vapor flooding limit and 50 % for the liquid flooding limit. The liquid flooding limit specification is available only if the downcomer geometry is specified. The allowable limit for liquid flooding (due to downcomer backup) can be specified on the Tray Rating|Downcomers block. For packed and tray columns, jet flooding controls the calculation of vapor flooding limits. For tray columns, parameters such as downcomer backup control the liquid flooding limits.

Results and discussion

Figure 2 displays the back-end separation of the ethylene plant considered in this study. Table 1 presents the base-case configurations for all the columns, which operate with large number of stages under high pressure, large reboiler duties, and large boilup rates. Column 3, especially, requires very large hot and cold utilities. The column

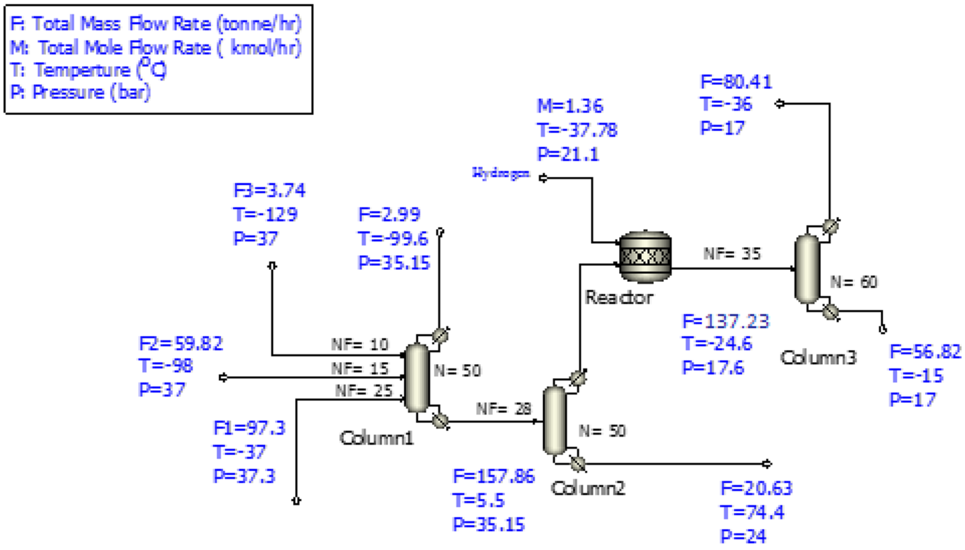
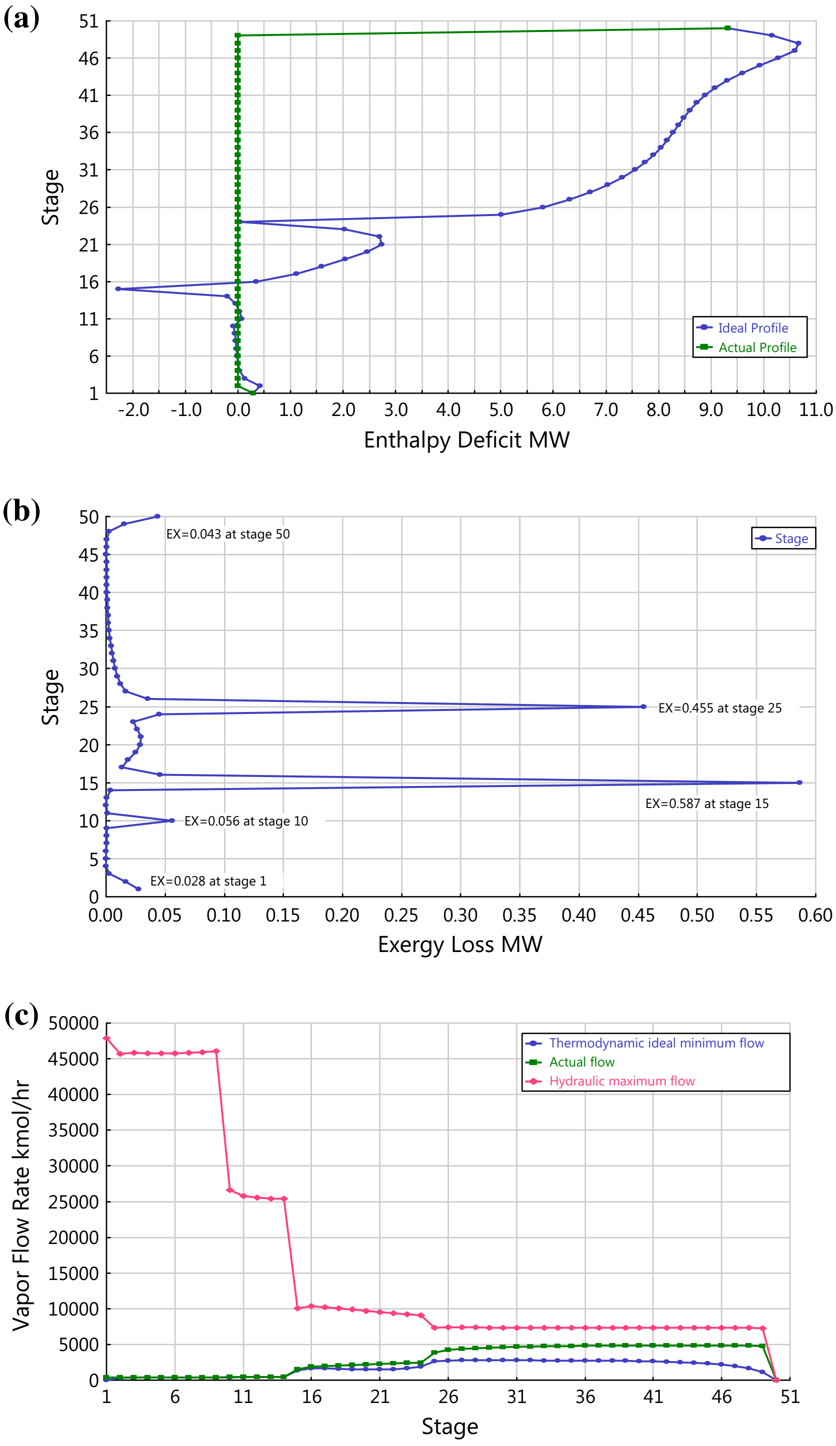


Fig. 2 Section of ethylene plant back-end separation; *N*: number of total stages; *NF*: feed plate location

Fig. 3 Base case operation for column 1 with: $N = 50$; $NF1 = 25$, $NF2 = 15$, $NF3 = 10$; $RR = 0.65$; N: number of total stages; $NF1$, $NF2$, $NF3$ are the feed stages, and RR is the reflux ratio. **a** CGCC (stage-H), **b** exergy loss profiles, and **c** hydraulic analysis



targeting tool with activated carbon tracking is used to reduce the duties for condensing and reboiling, stage exergy losses, as well as the carbon dioxide emissions due to the utilities for all the columns. The modified case operations with the determined scope of retrofits are compared with the base case operations to analyze and assess the impact of retrofits in the selected sustainability metrics.

Feed location modification

In the analysis, the condenser and reboiler are defined to be the first and last stages, respectively.

- If a feed is introduced too high up in the column, a sharp enthalpy change occurs on the condenser side on the stage-H CGCC plot; the feed stage should be moved down toward the reboiler.

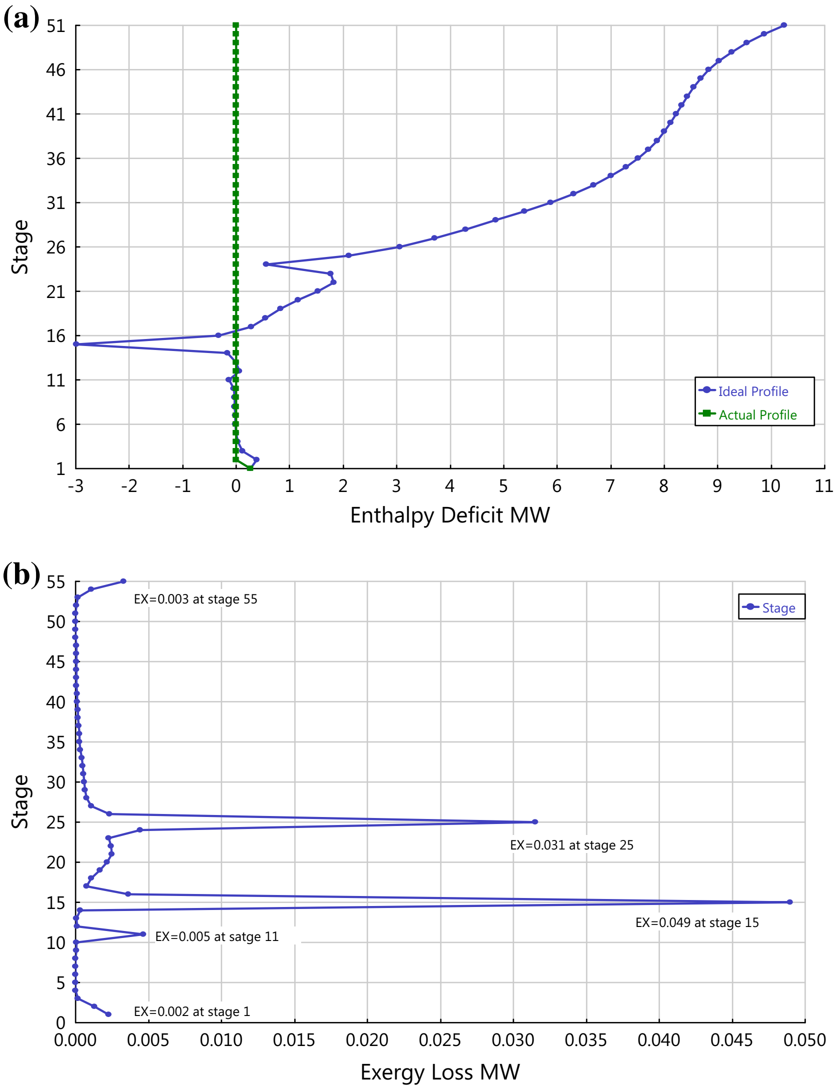


Fig. 4 Modified case operation for Column 1 with $N = 55$; $NF1 = 25$, $NF2 = 15$, $NF3 = 10 \rightarrow 11$; $RR = 0.38$; $TF1 = -37\ ^\circ\mathrm{C} \rightarrow -30\ ^\circ\mathrm{C}$; *N*, number of total stages; *NF1*, *NF2*, and *NF3* are the feed stages, and *RR* is the reflux ratio. **a** CGCC (stage-*H*), and **b** exergy loss profiles

- If a feed is introduced too low in the column, a sharp enthalpy change occurs on the reboiler side on the stage-*H* CGCC; the feed stage should be moved up toward the condenser [1, 10].

When the feed locations are appropriate, these distortions are less sharp and this may lead to reduced reboiler and condenser duties as well as exergy losses. However, in this case the modification of the feed plate location shows a negligible, or a very small reduction in column 1 duties and CO_2 emission but not the exergy loss, while no noticed reduction in column 2. On the other hand, column 3 modification shows reductions in duties and CO_2 emission. This will be discussed more in the scope of reflux ratio modification, which requires changing the number of total stages and the feed plate locations.

Feed conditioning modification

Feed conditioning is necessary when sharp enthalpy change in reboiler or condenser is noticed on the stage-*H* CGCC plot:

- If a feed is excessively sub-cooled, the stage-*H* plots show a sharp enthalpy changes on the reboiler side, and extent of this change determines the approximate feed heating duty required.
- If a feed is excessively over heated, the stage-*H* plots show a sharp enthalpy changes on the condenser side, and extent of this change determines the approximate feed cooling duty required.
- Changes in the heat duty of pre-heaters or pre-coolers lead to similar duty changes in the column reboiler or condenser loads, respectively [1].

Table 3 Sustainability metrics for column 1 with the modification: $N = 50 \rightarrow 55$; $NF1 = 25$, $NF2 = 15$, $NF3 = 11$; $RR = 0.65 \rightarrow 0.328$; $TF1 = -37\ °C \rightarrow -30\ °C$

	Column 1		
	Base case	Modified case	Change (%)
Material intensity			
Feed 1 rate (kg/s)	27.03	27.03	0
Feed 2 rate (kg/s)	16.62	16.62	0
Feed 3 rate (kg/s)	1.04	1.04	0
Distillate rate (kg/s)	0.83	0.83	0
Bottoms rate(kg/s)	43.85	43.85	0
Energy intensity metrics			
Condenser duty, kJ/s/(kg/s distillate), kJ/kg	−356.92	−345.67	−3.17
Reboiler duty, kJ/s/(kg/s bottoms), kJ/kg	212.71	199.99	−5.98
Feed conditioning, kJ/s/(kg/s feed 1), kJ/kg	0	20.28	–
Condenser duty cost, \$/s/(kg/s distillate), \$/kg	0.015	0.014	−3.12
Reboiler duty cost, \$/s/(kg/s bottoms), \$/kg	0.0007	0.0006	−5.97
Duty in feed 1 conditioning cost, kJ/s/(kg/s feed 1), \$/kg	0	0.00004	–
Total exergy loss, kJ/s/(kg/s ethylene), kJ/kg	70.98	5.56	−92.15
Environmental impact metrics			
Condenser CO_2 emission, kg/s/(kg/s distillate)[a]	0.0198	0.0191	−3.53
Reboiler CO_2 emission, kg/s/(kg/s bottoms)[a]	0.012	0.011	−8.33
Feed conditioning CO_2 emission, kg/s/(kg/s feed 1)[a]	0	0.001	–

[a] Emission based on US-EPA-Rule-E9-5711 and natural gas

Because of the large differences of the temperature in the distillate and bottom flows, feed conditioning does not give satisfactory retrofits for columns. Heating the feed reduces the heat duty and the CO_2 emission of the reboiler, but it increases them in the condenser. However, the feed conditioning represents better retrofits if applied with reflux ratio modification because reflux ratio modification decreases the duties and CO_2 emission in both sides. Detailed results will be presented and discussed in “Reflux ratio modification” section.

Reflux ratio modification

The gap between the pinch point and ordinate suggests that the duties in the reboiler and condenser can be further reduced by reducing reflux ratio [1]. However, to maintain the separation, the number of stages must increase. NQ curves analysis can be applied to find the optimum number of stages and the optimum feed stage based on an objective function, which may minimize total hot and cold duties or reflux ratio. The NQ curves are applied on columns with an objective function of minimizing the total duty (reboiler + condenser). To generate NQ curves, several steps should be considered: (1) specify the total number of stages, (2) activate design specifications such as purity, recovery, and/or stage temperature, (3) specify upper and lower limits for the number of stages, (4) select feed stage for the feed tray optimization, and (5) specify the objective function.

Side condensing or reboiling modification

Side condensing or side reboiling is external modification at a convenient temperature level. The area between the ideal and actual enthalpy (the CGCC pinch point) can be used to determine the scope for side condensing or side reboiling. This area could be reduced by integrating side condensing or reboiling, (or both in some cases) on an appropriate stage [1, 10, 18, 23].

- If a significant area exists above the pinch, a side reboiler can be placed at a convenient temperature level. This allows heat supply to the column using a low-cost hot utility, thus lowering the overall operating costs.
- If a significant area exists below the pinch, a side condenser can be placed at a convenient temperature level. This allows heat removal from the column more effectively and by a cheaper cold utility, thus lowering the overall operating costs.

In the next section, the determination of scope of retrofits and possible modifications are discussed for each column.

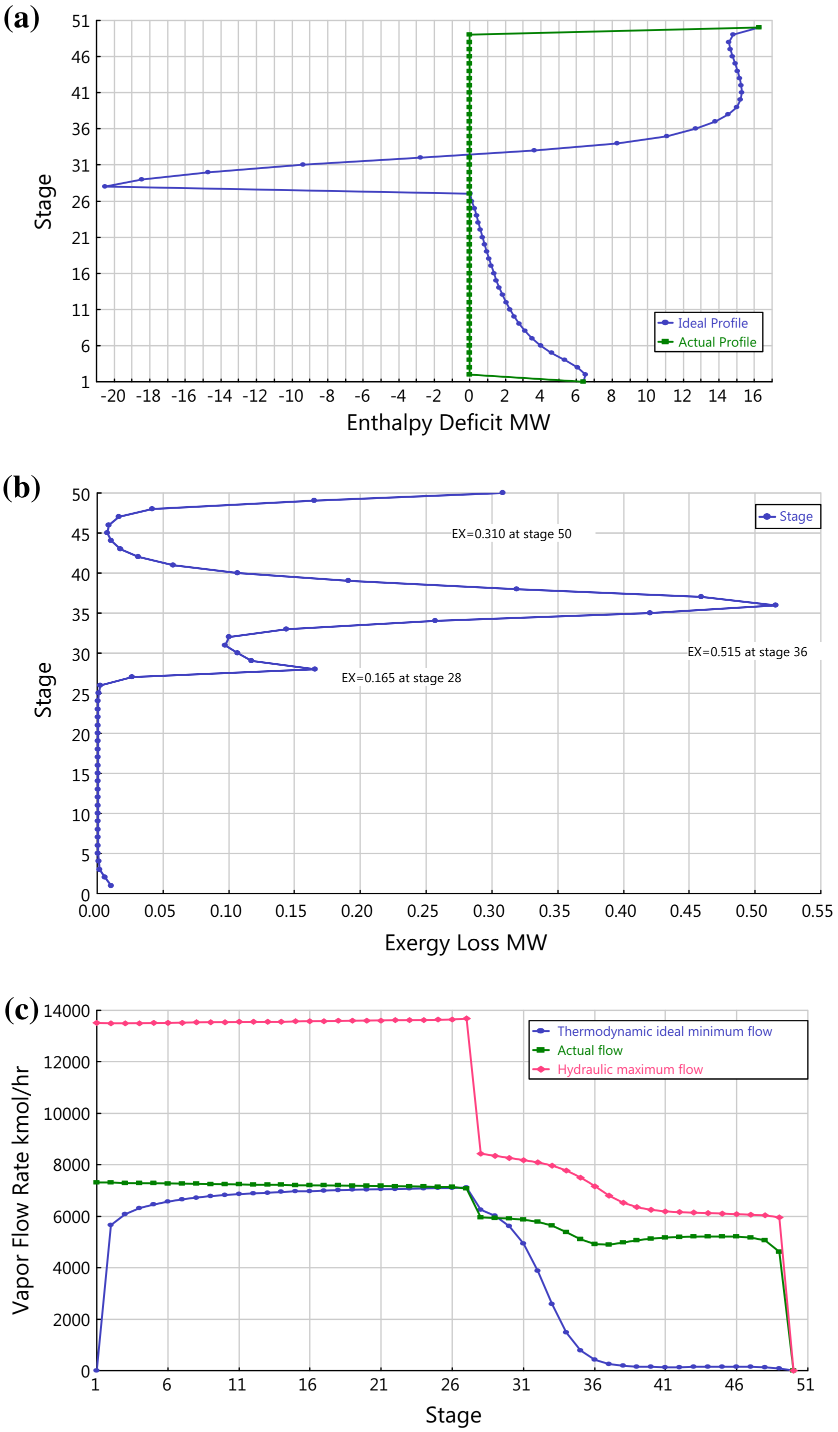


Fig. 5 Column 2 base case operation with $N = 50$; $NF = 28$; $RR = 0.53$; N, number of total stages; $NF1$, $NF2$, and $NF3$ are the feed stages, and RR is the reflux ratio. **a** CGCC (stage-H), **b** exergy loss profile, and **c** hydraulic analysis

Column 1

Table 1 shows that the first column operates with three feed streams under cryogenic conditions. Figure 3 shows the stage-*H* CGCC, exergy loss profiles, and hydraulic analysis for the base case operations

Stage-*H* CGCC shown in Fig. 3a displays sharp changes for the feeds 2 and 3 on the condenser side, which require moving the feeds up the column toward condenser. Also, it displays sharp enthalpy change on the reboiler side, which requires heating the first feed. Therefore, the first feed has been heated to −30 °C instead of −37 °C. The small gap

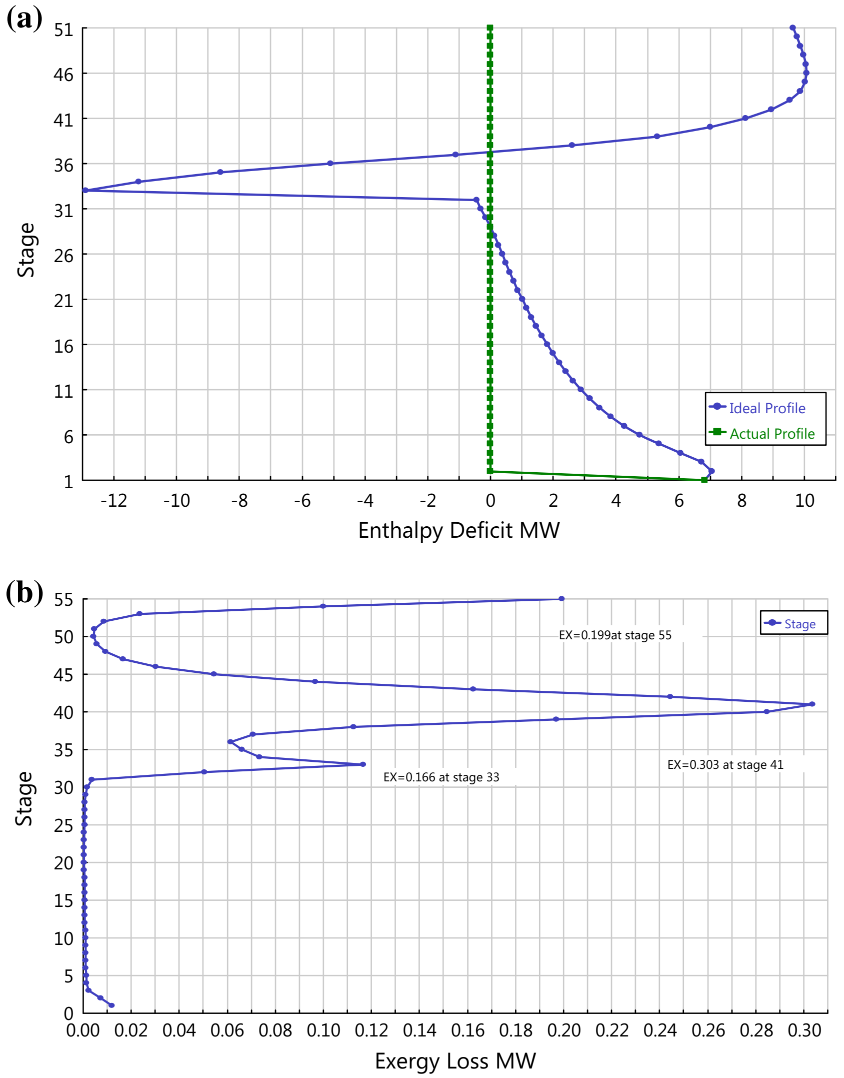


Fig. 6 Modified case operation for column 2 with $N = 55$; $NF = 33$; $RR = 0.53$; N, number of total stages; NF is the feed stage, and RR is the reflux ratio. **a** CGCC (stage-H), and **b** exergy loss profiles

to the ordinate requires a reflux ratio modification which leads to changing in the number of stages. Therefore; NQ curve analysis is used to get 55 stages with reflux ratio of 0.38, and the third feed is moved up the column for the $NF3$ to be 11. Exergy loss profile shown in Fig. 3b displays the wasted available energy in the column and higher exergy losses on the feed stages, the reboiler, and the condenser. Figure 3c displays the vapor flow rate profile, which is near minimum in the feed stages and the reboiler and near maximum in the condenser. The supporting data show some of the data obtained from the NQ curve analysis.

NQ curves are applied for column 1 with $N = 55$; $NF1 = 25$, $NF2 = 15$, $NF3 = 11$, and $RR = 0.32$, where N is the number of total stages, $NF1$, $NF2$, and $NF3$ are the feed stages, and RR is the reflux ratio. The results of NQ curve are presented in Table S5 within the supplementary data. Figure 4a displays the modified CGCC (stage-H) with relatively less heat deficits around the feed stages. Figure 4b shows the exergy loss profiles of the column after the modifications. The total metrics of exergy losses on the feed stages are reduced from the base case of operation value of 70.98–5.57 kW per kg/s ethylene after the modifications. Therefore, the total reduction is around 92 %. The hydraulic analysis shows that the changes in the internal vapor flow rates are negligible.

Table S5 in supplementary data compares the sustainability indicators, while Table 3 compares the sustainability metrics, which are normalized values with respect to unit mass of products for both the base case and modified case operations. The modifications applied are the reflux ratio, feed plate location, and heating feed 1 of column 1. As seen, the modification have resulted in modest reductions in the duties, the cost of energy, and emissions of CO_2, while reducing the exergy losses considerably. The emission calculations are based on CO_2 emission factor

Table 4 Sustainability metrics for column 2 with the modifications: $N = 50 \rightarrow 55$; $NF = 33$; $RR = 0.65 \rightarrow 0.53$; $TF = 5\ °C \rightarrow 9\ °C$

	Column 2		
	Base case	Modified case	Change (%)
Material intensity			
Feed rate (kg/s)	43.85	43.85	0
Distillate rate (kg/s)	38.12	38.12	0
Bottoms rate(kg/s)	5.73	5.73	0
Energy intensity metrics			
Condenser duty, kJ/s/(kg/s distillate), kJ/kg	−167.49	−179.41	+6.63
Reboiler duty, kJ/s/(kg/s bottoms), kJ/kg	2837.58	1941.14	−31.60
Feed conditioning, kJ/s/(kg/s feed), kJ/kg	0	127.51	–
Condenser duty cost, \$/s/(kg/s of distillate), \$/kg	0.0019	0.0021	+6.63
Reboiler duty cost, \$/s/(kg/s bottoms), \$/kg	0.0054	0.0038	−31.60
Duty in feed conditioning cost, kJ/s/(kg/s feed), \$/kg	0	0.0002	–
Total exergy loss, kJ/s/(kg/s ethylene), kJ/kg	166.86	104.94	−37.10
Environmental impact metrics			
Condenser CO_2 emission, kg/s/(kg/s distillate)[a]	0.009	0.01	+10.00
Reboiler CO_2 emission, kg/s/(kg/s bottoms)[a]	0.16	0.11	−31.25
Feed conditioning CO_2 emission, kg/s/(kg/s feed)[a]	0	0.007	–

[a] Emission based on US-EPA-Rule-E9-5711 and natural gas

data source of US-EPA-Rule-E9-5711 and natural gas as the fuel source. Besides, the exergy loss is reduced by around 92 % after the modifications leading to efficiently usage of available energy and more thermodynamically optimum operation.

Reflux ratio and number of stages modifications have no impact on the bottoms flow rate and compositions of column 1. This means that there is no impact on column 2 after column 1 reflux ratio and number of stages modifications.

Column 2

For the base case operation of column 2, which is summarized in Table 1, Fig. 5 shows CGCC (stage-*H*), exergy loss profiles, and hydraulic analysis. Figure 5a displays a sharp enthalpy change close to the reboiler side, which means that the feed heating may improve the operation. Also, reflux ratio modification may be required to further reduce the small gap to the ordinate. Figure 5b shows that the exergy loss is higher in the feed stage, stage 36, and stage 55. As Fig. 5c shows that the vapor flow rate is near minimum on the feed stage.

Using the NQ curves approach, which is available in supplementary data in Table S6; column 2 has been modified with $N = 55$; $NF = 33$; $RR = 0.53$, where N is the number of total stages, NF is the feed stages, and the RR is the reflux ratio. Figure 6a shows that the deficit at the feed stage has been reduced considerably on the CGCC (stage-*H*) after changing the number of stages and heating the feed up to 9 °C. Figure 6b shows considerable reduction of around 37 % in the exergy losses with the modified operations. The hydraulic analysis the vapor flow rate profiles are negligible after the modification.

Table S3, available in supplementary data, compares the sustainability indicators before and after modifications. Table 4 compares the sustainability metrics for the base case and modified case operations for column 2. As seen, the duties and cost of energy are decreased in the reboiler side, while the condenser duty is increased due to heating the feed. In a similar trend, the emissions of CO_2 decreased around 31.6 % in the reboiler, while increased around 6.6 % in the condenser. This indicates the tradeoff taking place during the modifications. The reduced exergy losses lead to a more thermodynamically optimum operation.

Column 3

Column 3 uses the distillate rate of column 2 as the feed. Table 4 shows that distillate rate of column 2 remains the same after the modifications; therefore, column 3 base case does not change after the modifications on column 2. For the base case operation of column 3, Fig. 7 shows the stage-*H* CGCC, exergy loss profiles, and hydraulic analysis. Figure 7a shows that the gap between the ordinate and the composite curve should to be reduced by modifying the reflux ratio. Figure 7b displays large exergy losses on stages 23 and 41. The vapor flow rate (shown in Fig. 8c) reaches hydraulic maximum flow in stage 61.

Using the NQ curve approach (see Table S7 in supplementary data), column 3 has been modified with $N = 66$; $NF = 35$; and $RR = 4.49$. Figure 8 shows the CGCC

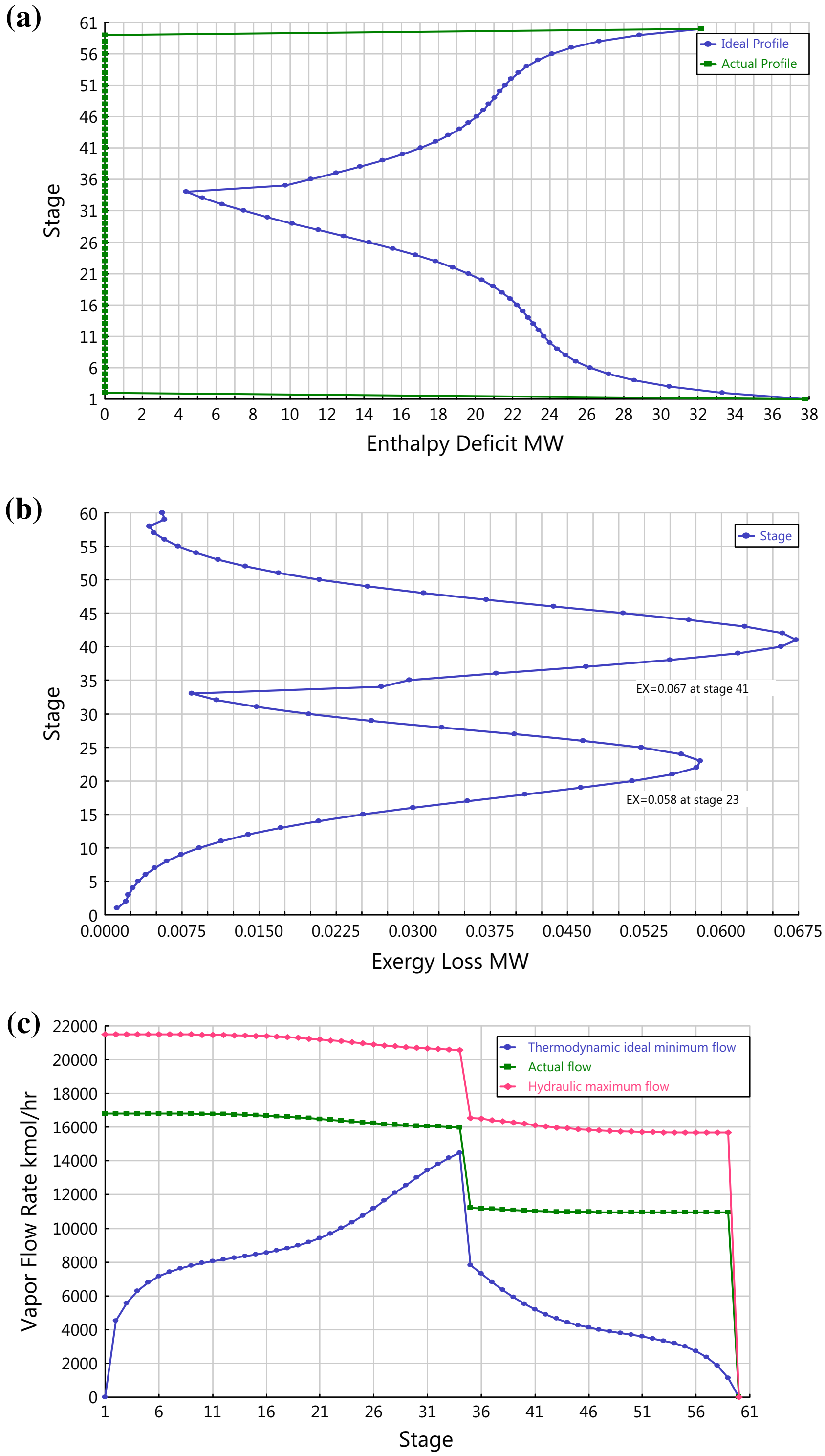


Fig. 7 Column 3 base case operation with $N = 60$; $NF = 35$; $RR = 4.75$; N, number of total stages; NF is the feed stages, and RR is the reflux ratio. **a** CGCC (stage-H), **b** exergy loss profile, and **c** hydraulic analysis

(stage-H) and exergy profiles after these modifications. The change in hydraulic analysis is negligible. Tables S4 and S5 in supplementary data compare the sustainability indicators and metrics, respectively, for the base case and modified case operations. The reduction in energy usage, energy cost, and exergy losses are achieved after the modifications. The sustainability metrics, shown in Table 5, indicate that the total exergy losses and total CO_2 emissions are reduced around 17.4 and 20 %, respectively.

The side reboiling or condensing is the modification which is not applied in this study because it does not show the desired results.

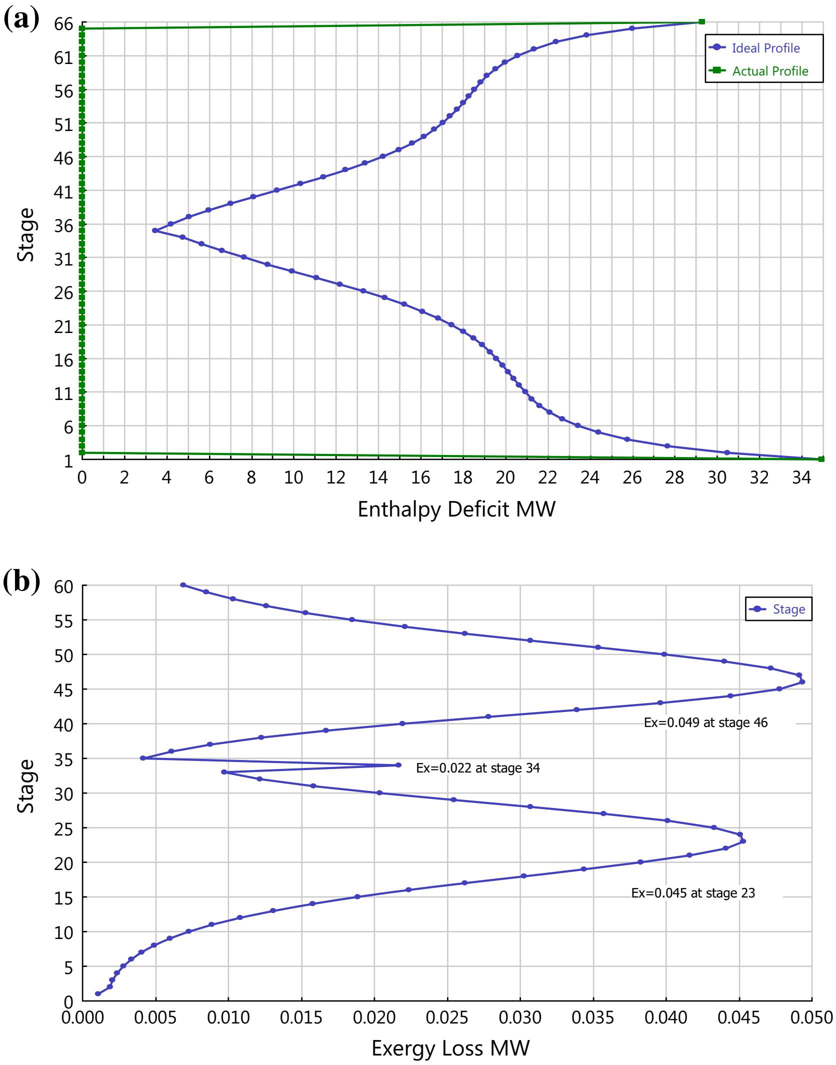


Fig. 8 Modified case operation for column 3 with $N = 66$; $NF = 35$; $RR = 4.49$; N, number of total stages; NF is the feed stage, and RR is the reflux ratio. **a** CGCC (stage-H), and **b** exergy loss profiles

Table 5 Sustainability metrics for column 3 with modifications: $N = 66$; $NF = 35$; $RR = 4.49$

	Column 3		
	Base case	Modified case	Change (%)
Material intensity			
Feed rate (kg/s)	38.12	38.12	0
Distillate rate (kg/s)	22.33	22.33	0
Bottoms rate (kg/s)	15.78	15.78	0
Energy intensity metrics			
Condenser duty, kJ/s/(kg/s distillate), kJ/kg	−1692.98	−1570.57	−7.23
Reboiler duty, kJ/s/(kg/s of bottoms), kJ/kg	2039.87	1845.17	−9.54
Condenser duty cost, \$/s/(kg/s of distillate), \$/kg	0.0286	0.0266	−7.22
Reboiler duty cost, \$/s/(kg/s of bottoms), \$/kg	0.0065	0.0058	−9.58
Total exergy loss, kJ/s/(kg/s ethylene), kJ/kg	75.29	62.18	−17.40
Environmental impact metrics			
Condenser CO_2 emission, kg/s/(kg/s distillate)[a]	0.09	0.08	−11.11
Reboiler CO_2 emission, kg/s/(kg/s bottoms)[a]	0.11	0.10	−9.09

[a] Emission based on US-EPA-Rule-E9-5711, natural gas

Table 6 Estimated efficiencies and energy savings for the three columns

System	Base case			Modified case						
	Ex_{min} (MW)	Ex_{loss} (MW)	η (%)	Ex_{min} (MW)	Ex_{loss} (MW)	η (%)	Saved Ex_{loss} (MW)	Change Ex_{loss} (%)	FCC of retrofits $[a]	Electricity saving ($/year)[b]
Column 1	−2.63	1.58	62.4	−2.48	0.12	95.2	1.46	92.2	100,600	964,038
Column 2	−1.72	3.73	31.5	−1.69	2.34	41.9	1.38	37.1	186,000	911,214
Column 3	0.77	1.68	31.4	0.97	1.39	41.0	0.29	17.1	338,000	191,487
Total		6.99			3.85		3.14		624,600	2,066,739

Ex_{loss}: total column exergy loss from the converged simulation by Aspen Plus with the SRK method

[a] *FCC* fixed capital cost

[b] Electricity equivalent of energy saving is based on a unit cost of electricity of $0.0775/kW-h

Table 7 Estimated total reductions in hot and cold duties for the three columns

System	Base case		Modified case		
	Condenser (MW)	Reboiler (MW)	Condenser (MW)	Reboiler (MW)	Feed conditioning (MW)
Column 1	−0.29	9.32	−0.28	8.769	0.54
Column 2	−6.38	16.26	−6.83	11.123	5.59
Column 3	−37.81	32.19	−35.08	29.125	–
Total	−44.49	57.78	−42.20	49.018	6.13

Table 8 Estimated total reductions in CO_2 emissions for the three columns

System	Base case CO_2 emissions (kg/s)	Modified case CO_2 emissions (kg/s)
Column 1	0.538	0.506
Column 2	1.265	1.004
Column 3	3.913	3.588
Total	5.716	5.098

Table 6 shows the estimated thermodynamic efficiency and the energy savings based on electricity, which is around $2 million against the fixed capital cost of around $624,600 (2014 U.S. $). This considerable energy saving, especially from reduction in exergy losses, also leads to the considerable CO_2 reductions as shown in Tables 7 and 8; the total reductions in the cold utility is around is 5.1 %, while the total reductions in the hot utility is around 4.5 %.

Table 8 shows that the total reductions in the emission of CO_2 are around 19.0 %. Table 9 shows the approximate total capital costs of $666,800 for the retrofits against the total energy savings in electricity of around $2,066,739. The hot utility for the feed conditioning of columns 1 and 2 has been counted in Table 9.

Conclusions

As distillation columns are highly energy-intensive processes, tools for reducing the energy consumptions, and hence the carbon emissions through reasonable retrofits are highly valuable for petrochemical industry. One such tool, based on the thermodynamic analysis, is the column targeting tool (CTT) with capabilities of thermal and hydraulic analyses. By using the CTT, it is possible to assess the operations with the current configurations and

Table 9 Approximate total costs of the retrofits and duty

Retrofits	Type	Duty (kW)	*P* (bar)	Material	Area (m^2)	Total cost ($)
Col. 1 heater	S/T fixed[a]	550.0	36.88	Carbon steel	4.40	9900
Col. 1 retrofit						110,500
Col. 2 heater	S/T fixed[a]	5590.0	34.47	Carbon steel	60.17	11,200
Col. 2 retrofit						197,200
Col. 3 retrofit						338,000
Total						666,800

[a] S/T: fixed shell and tube

determine the possible scope for improvements in modified configurations by suitable retrofits. Best possible column retrofits may be obtained by using the modifications on feed conditioning, feed stage, and reflux ratio. This analysis also includes the carbon tracking using an appropriate standard and a primary fuel. Using thermodynamic analysis, higher thermodynamic efficiencies are obtained for all the three columns, and the energy savings due to these modifications are about \$2 millions/year (2014 U.S. \$) after a one-time fixed capital cost of \$664,000. The reduction in total hot and cold utilities is around 10 %. Besides, the reduction in carbon emission is around 14 %. The results illustrate that it may be possible to achieve an improved and more sustainable distillation operation by simple retrofits determined by thermodynamic analysis.

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Authors' contributions Both authors, MA and YD, contributed equally in writing the paper. Both authors read and approved the final manuscript.

Compliance with ethical standards

Conflict of interest The authors declare that they have no competing interests.

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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.

	Column 1		Column 2		Column 3	
Operation	Base	Modified	Base	Modified	Base	Modified
N	50	55	50	55	60	66
NF	NF1=25 NF2=15 NF3=10	NF1=25 NF2=15 NF3=11	28	33	35	35
Mole RR	0.65	0.33	0.54	0.53	4.75	4.49
F (mt/hr)	F1=97.3 F2=59.82 F3=3.74	F1=97.3 F2=59.82 F3=3.74	175.86	175.86	173.23	173.23
P (bar)	35.15	35.15	23.9	23.9	16.87	16.87
TF (ºC)	TF1= −37 TF2= −98 TF3= −129	TF1= −30 TF2= −98 TF3= −129	5	9	−24.6	−24.6
PF (bar)	PF1=37.3 PF2=37 PF3=37	PF1=37.30 PF2=37 PF3=37	35.15	35.15	17.6	17.6
Condenser duty (MW)	−0.29	−0.55	−6.38	−8.22	−37.81	−40.30
Condenser temp.(ºC)	−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	137.231	137.23	80.41	80.41
Reboiler duty (MW)	9.33	9.68	16.26	18.09	32.2	34.34
Reboiler temp.(ºC)	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.

	Column 1		
Material intensity indicators	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	–

[1] Emission 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.

	Column 2		
Material intensity indicators	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	–

[1] Emission 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.

	Column 3		
Material intensity indicators	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

[1] Emission 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

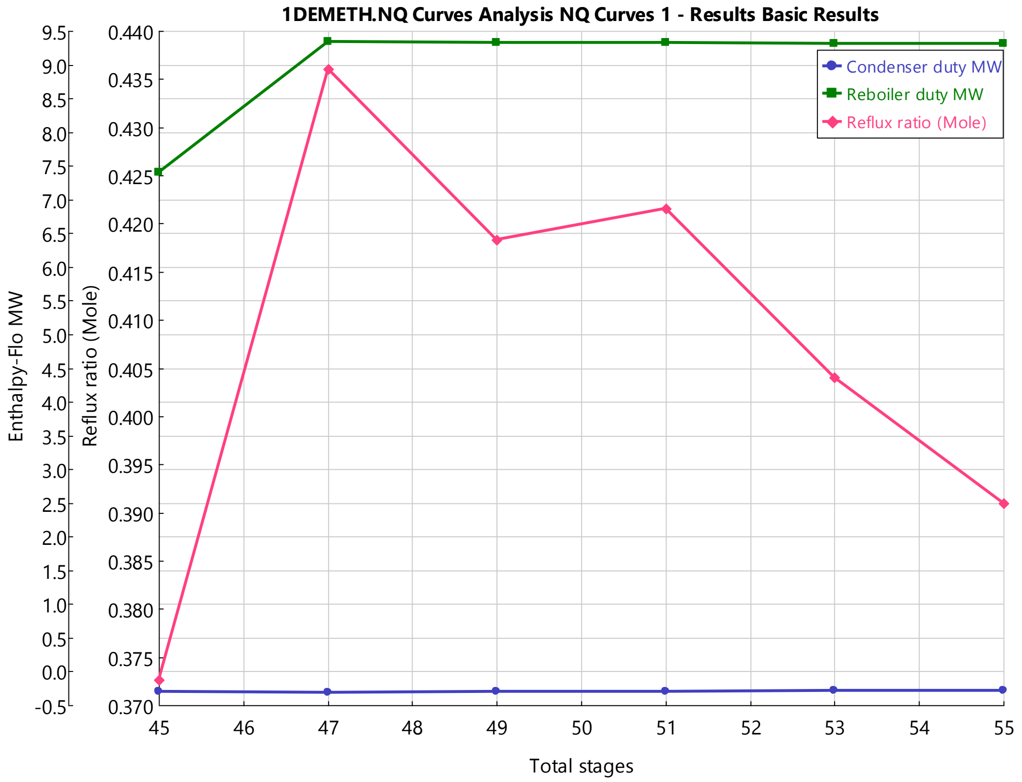

Fig. S1. Column 1 NQ curve curves results.

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

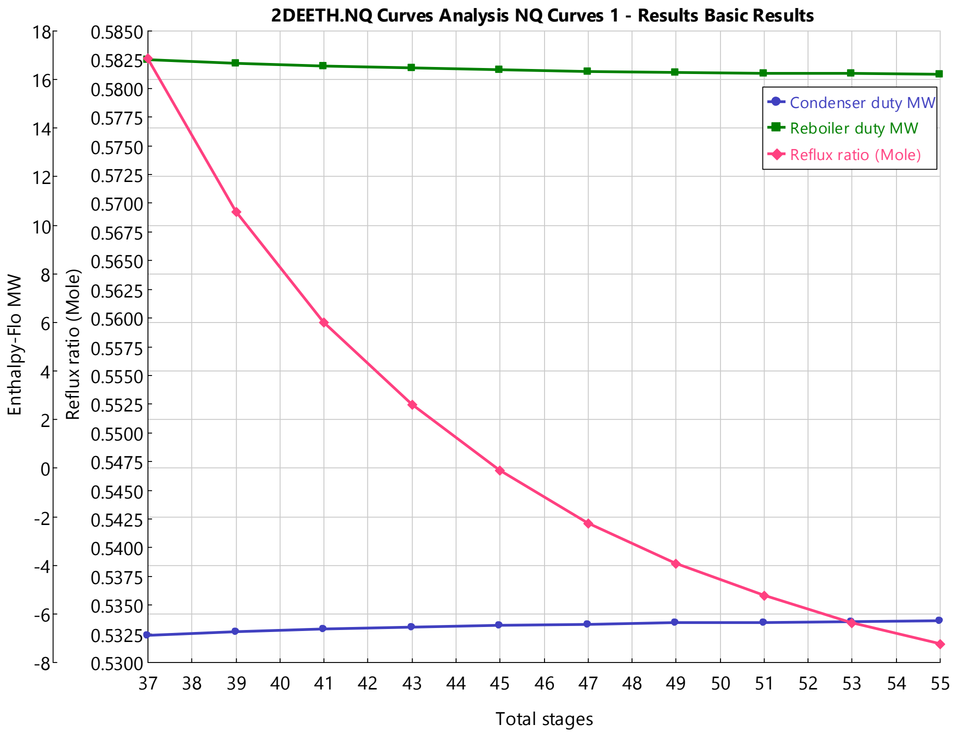

Fig. S2. Column 2 NQ curve curves results.

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-l) 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

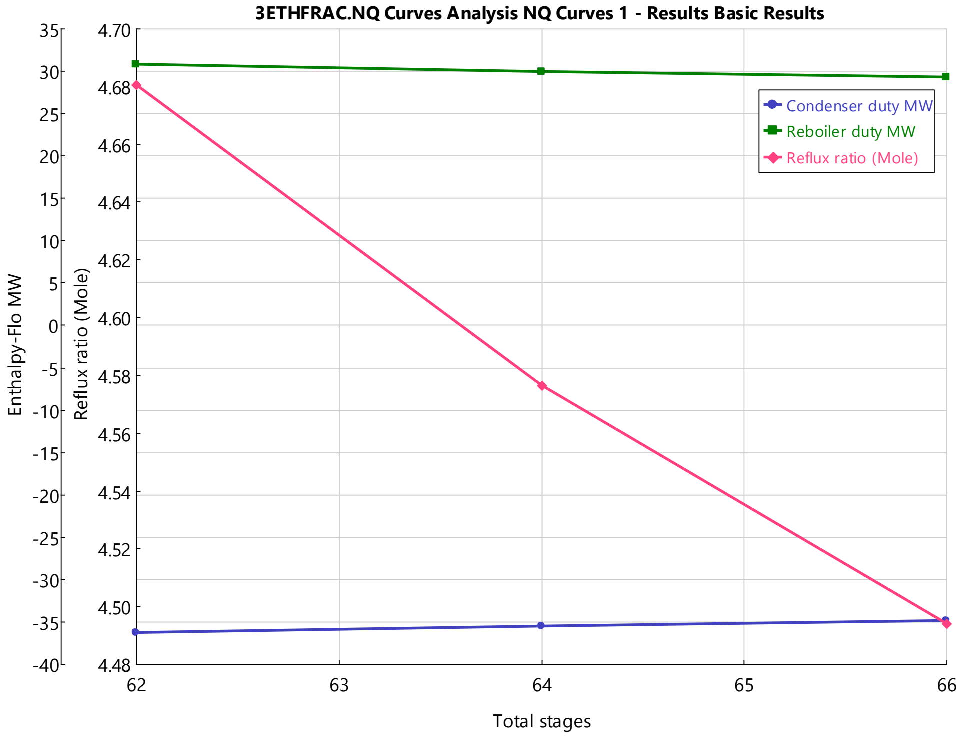

Fig. S3. Column 3 NQ curve curves results.

Utility Price:

Table S**8**
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.

	Base Case			Modified Case		
Column 1	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 CO_2 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, ºC	-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, ºC	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, ºC	-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