SciMedCentral Chemical Engineering & Process Techniques

Research Article

Sustainable Operations for Distillation Columns

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Submitted: 17 July 2013
Accepted: 07 August 2013
Published: 09 August 2013

Keywords
- Sustainability metrics
- Distillation column
- Column targeting tool
- Column grand composite curves
- Carbon tracking; Global warming potential

Abstract

Distillation process consumes about 40% of the total energy used to operate the plants in petrochemical and chemical process industries in North America. Therefore, sustainable distillation column operation requires responsible use of energy and reduction of harmful emission such as CO_2. The Aspen Plus 'Column Targeting Tool' (CTT) options in a simulation environment can help reduce the use of energy and hence CO_2 emission. The Aspen plus 'Carbon Tracking' (CT) together with the 'Global Warming Potential' options can quantify the reduction in CO_2 emission. The CTT is based on the practical near-minimum thermodynamic condition approximation and exploits the capabilities for thermal and hydraulic analyses of distillation columns to identify the targets for possible column modifications. By using the 'CO_2 emission factor data source' and fuel type, the CT estimates the total CO_2 emission and net carbon fee/tax in the use of utility such as steam. A comparative assessment with the sustainability metrics displays the usage of energy, emission of CO_2, and cost before and after the distillation column modifications. This study comprises both an interactive and graphically-oriented case study with simulation tool and sustainability metrics for quantifying the reduction in the energy consumption and CO_2 emission in distillation column operations.

INTRODUCTION

The U.S. Department of Energy estimates that there are more than 40,000 distillation columns consuming about 40% of the total energy used to operate the plants in petrochemical and chemical process industries in North America [1,2]. A typical distillation column resembles a heat engine 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 [3]. Aspen Plus 'Column Targeting Tool' (CTT) is based on the Practical Near-Minimum Thermodynamic Condition (PNMTC) approximation representing a practical and close to reversible operation [4-9]. It exploits the capabilities for thermal and hydraulic analyses of distillation columns to identify the targets for possible column modifications in: 1) stage feed location, 2) reflux ratio, 3) feed conditioning, and 4) side condensing and/or reboiling. These modifications can reduce the utility usage and improve energy efficiency.

The options of CTT can help reduce the use of energy, while the 'Carbon Tracking' (CT) and Global Warming Potential options can help quantify the reduction in CO_2 emission in a simulation environment. If nonrenewable and limited, energy usage affects environment through the emission of pollutants such as CO_2. Sustainability has environmental, economic, and social dimensions and requires the responsible use of resources such as energy and reduction in CO_2 emission. The three intersecting dimensions illustrate sustainability metrics (3D) that include material use, (nonrenewable) energy use, and toxic and pollutant emissions [10-14]. In this study, the energy and CO_2 emission as the pollutant are used as the sustainability metrics in distillation column operations. This study demonstrates how to reduce and quantify the energy consumption and CO_2 emissions with the sustainability metrics in distillation column operations.

MATERIALS AND METHODS

Sustainability

'Sustainability is maintaining or improving the material and social conditions for human health and the environment over time without exceeding the ecological capabilities that support them [6]'. The dimensions of sustainability are economic, environmental, and societal (Figure 1). 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 that are quantifiable and applicable to a specific process [15,16]

- Material intensity (nonrenewable resources of raw materials, solvents/unit mass of products)
- Energy intensity (nonrenewable energy/unit mass of products)
- Potential environmental impact (pollutants and

Cite this article: *Demirel Y (2013) Sustainable Operations for Distillation Columns. Chem Eng Process Tech 1: 1005.*

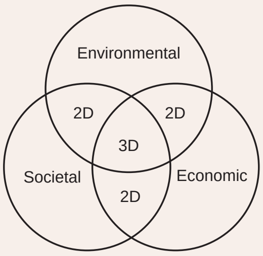


Figure 1 Three dimensions of sustainability.

emissions/unit mass of products)

- Potential chemical risk (toxic emissions/unit mass of products)

The first two metrics are associated with the process operation. The remaining two metrics represent chemical risk to human health in the process environment, and the potential environmental impact of the process on the surrounding environment. For distillation column operations, this study uses a comparative assessment with the sustainability metrics of:

- ‘Energy intensity’ as nonrenewable energy/unit mass of products by using ‘Column Targeting Tool.’
- ‘Potential environmental impact’ as emissions and cost/unit mass of products by using ‘Carbon Tracking’ and ‘Global Warming Potential’ options of the Aspen Plus simulator.

Column targeting tool

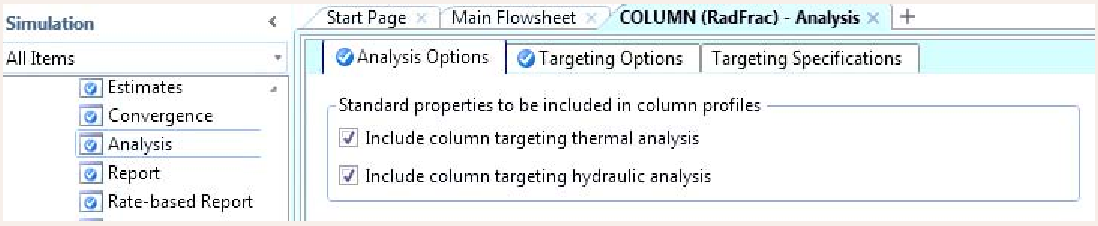
The Column Targeting Tool (CTT) of Aspen Plus is a conceptual design tool for lowering cost of operation through modified operating conditions, and providing insight into understanding tray/packing capacity limitations. The CTT is based on the Practical Near-Minimum Thermodynamic Condition (PNMTC) representing a close to practical reversible column operation [10]. For RadFrac, MultiFrac, and PetroFrac column models, the CTT performs thermal, exergy, and hydraulic analyses capabilities that can help identify the targets for appropriate column modifications in order to [7,14,17].

- Reduce utilities cost
- Improve energy efficiency
- Reduce capital cost by improving thermodynamic driving forces
- Facilitate column debottlenecking

The CTT can be activated by using the corresponding option on the Analysis / Analysis Options sheets, as shown in (Table 1). Results of the column targeting analysis depend strongly on the selection of light key and heavy key components in Targeting Options (Table 2) [7]. Before designating light key and heavy components for the column (see Table 3), the user runs the simulation and inspects the column split-fractions, composition profiles, and component K-values displayed by the ‘Plot Wizard.’ If there is more than one light key component, the heaviest of them is selected as the light key. In case of multiple heavy key components, the lightest is selected as the heavy key. In the default method, key components are selected based on the component K-values. The CTT has a built-in capability to select light and heavy key components for each stage of the column [7].

Thermal analysis

Thermal analysis capability is useful in identifying design targets for improvements in energy consumption and efficiency [7,11-14,18-20]. In this capability the reboiling and condensing loads are distributed over the temperature range of operation of the column. The thermal analysis of CTT produces ‘Column

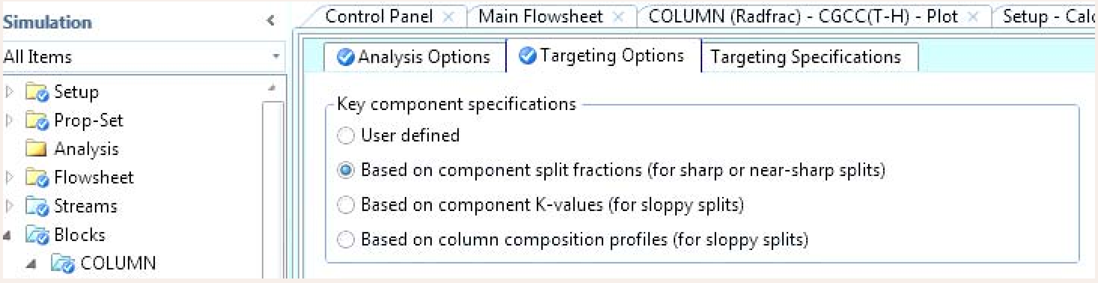


Standard properties to be included in column profiles

☑ Include column targeting thermal analysis

☑ Include column targeting hydraulic analysis

Table 1 Analysis / Analysis Options to activate the Column Targeting Tools (CTT).



Key component specifications

○ User defined

● Based on component split fractions (for sharp or near-sharp splits)

○ Based on component K-values (for sloppy splits)

○ Based on column composition profiles (for sloppy splits)

Table 2 Analysis / Targeting Options with key component specification.

Method	Use When
User defined	Allows you to specify the light key and heavy key components.
Based on component split-fractions	This method is best for sharp or near-sharp splits fractions in product streams.
Based on component K-values	This method is best for sloppy splits.
Based on column composition profiles	In principle, this method is similar to the K-value based method. It is best suited for sloppy splits and it is, in general, inferior to the K-value based method.

Table 3: Selection of key components within the 'Targeting Options' [7].

Grand Composite Curves' (CGCC) and 'Exergy Lost Profiles.' The user makes changes to column specifications until the profiles look right based on the column targeting methodology. The CGCCs are displayed as the stage-enthalpy (Stage-H) or temperature-enthalpy (T-H) profiles. 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 pressure drops, multiple side-products, and side strippers. The CGCCs are helpful in identifying the targets for potential column modifications for

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

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 by

$$H_{\text{Vmin}} = H_V^* \left(\frac{V_{\min}}{V^*} \right); \; H_{\text{Lmin}} = H_L^* \left(\frac{L_{\min}}{L^*} \right) \tag{1}$$

where V^* and L^* are the molar flows of equilibrium, H_V^* and H_L^* are the enthalpies of equilibrium vapor and liquid streams leaving the same stage, respectively, and the minimum vapor and liquid flow rates leaving the same stage with the same temperatures can be estimated by [13,14,18-20]

$$V_{\min} = \frac{1}{y_L^*}(D_L + L_{\min} x_L^*) \; ; \; L_{\min} = \frac{1}{x_H^*}(V_{\min} y_H^* - D_H) \tag{2}$$

From the enthalpy balances at each stage, the net enthalpy deficits are obtained by

$$H_{\text{def}} = H_{\text{Lmin}} - H_{\text{Vmin}} + H_D \quad \text{(Before the feed stage)} \tag{3}$$

$$H_{\text{def}} = H_{\text{Lmin}} - H_{\text{Vmin}} + H_D - H_{\text{feed}} \quad \text{(After the feed stage)} \tag{4}$$

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. At the feed stage, mass and energy balances differ from an internal stage and the enthalpy deficit at the feed stage becomes

$$\begin{aligned} H_{\text{def,F}} = Q_C + D[H_D + H_L(x_D - y_F^*) / \\ (y_F^* - x_F^*) - H_V(x_D - x_F^*) / (y_F^* - x_F^*)] \end{aligned} \tag{5}$$

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 pinch may exist in rectifying and stripping sections. Exergy (Ex) is defined the maximum amount of work that may be performed theoretically by bringing a resource into equilibrium with its surrounding through a reversible process.

$$Ex = \Delta H - T_o \Delta S \tag{6}$$

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. 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 [11,12,17]. Exergy balance for a steady state system is

$$\sum_{\substack{\text{into} \\ \text{system}}} \left[\dot{n}Ex + \dot{Q}\left(1 - \frac{T_o}{T_s}\right) + \dot{W}_s \right] - \sum_{\substack{\text{out of} \\ \text{system}}} \left[\dot{n}Ex + \dot{Q}\left(1 - \frac{T_o}{T_s}\right) + \dot{W}_s \right] = \dot{E}x_{\text{loss}} \tag{7}$$

Where $\dot{W}_s$ is the shaft work? As the exergy loss increases, the net heat duty has to increase to enable the column to achieve a required separation. Consequently, smaller exergy loss means less waste energy. The exergy profiles are plotted as state-exergy loss or temperature-exergy loss. In general, the exergy loss profiles can be used as a tool to examine the degradation of accessible work due to [7,11,12].

- Momentum loss (pressure driving force)
- Thermal loss (temperature driving force)
- Chemical potential loss (mass transfer driving force)

Hydraulic analysis

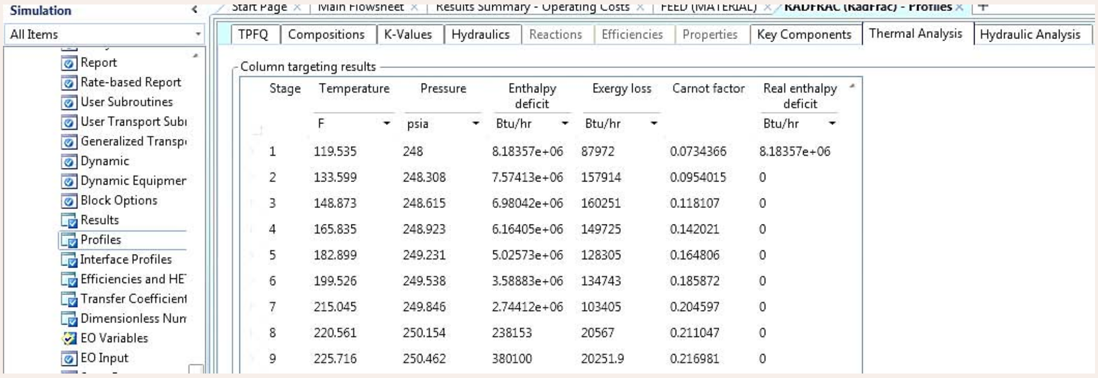
Tray or packing rating information for the entire column is necessary to activate the hydraulic analysis. In addition, allowable flooding factors (as fraction of total flooding) for flooding limit calculations can be specified. Hydraulic analysis helps identify the allowable limit for vapor flooding on the Tray Rating Design/Pdrop or Pack Rating|Design/Pdrop sheets. 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 down comer geometry is specified. The allowable limit for liquid flooding (due to down comer backup) can be specified on the Tray Rating|Downcomers sheet [7,13,14]. The hydraulic analysis capability helps 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. 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. Hydraulic analysis produces plots for flow rates versus stage and can be used to identify and eliminate column bottlenecks [7]. Graphical and tabular profiles (Table 4) help identifying targets and analysis for possible modifications by the user. The 'Plot Wizard' (Figure 2) produces various plots including the types:

- Thermal analysis: The CGCC (T-H) Temperature versus Enthalpy
- Thermal analysis: The CGCC (S-H) Stage versus Enthalpy
- Hydraulics analysis: Thermodynamic Ideal Minimum Flow, Hydraulic Maximum Flow, Actual Flow
- Exergy loss profiles: Stage versus Exergy Loss or Temperature versus Exergy Loss

RESULTS AND DISCUSSIONS

Sustainable column operation is illustrated in the following example using a RADFRAC column (Figure 3), which will be the base case. The input summary showing the feed flow rate, feed composition, column configuration, and utility bloc definitions are given below.

COMPONENTS: C2H6 C2H6 / C3H8 C3H8 / C4H10-1 C4H10-1 / C5H12-1 C5H12-1 / C6H14-1 C6H14-1 / WATER H2O PROPERTIES RK-SOAVE STREAM FEED: TEMP=225°F PRES=250 psia; MOLE-FLOW C2H6 30 / C3H8 200 / C4H10-1 370 / C5H12-1 350 / C6H14-1 50 lbmol/hr BLOCK RADFRAC RADFRAC: NSTAGE=14;CONDENSER=PARTIAL-V; FEED 4 PRODUCTS BOT 14 L / DIS 1 V; P-SPEC 1 248 psia COL-SPECS D:F=.226 MOLE DP-COL=4 MOLE-RR=6.06 TRAY-SIZE 1 2 13 SIEVE , TRAY-RATE 1 2 13 SIEVE DIAM=5.5 ft UTILITIES COND-UTIL=CW REB-UTIL=STEAM UTILITY Water; COST = 0.05 $/ton ; PRES=20. PRES-OUT=20. psia; TIN=50. TOUT=75. F UTILITY STEAM; COST =6. $/ton ; STEAM HEATING-VALU=850.0 Btu/lb CALCCO2=YES FACTORSOURCE="US-EPA-Rule-E9-5711" FUELSOURCE= "Natural gas" CO2FACTOR=1.30000000E-4



Column targeting results

Stage	Temperature	Pressure	Enthalpy deficit	Exergy loss	Carnot factor	Real enthalpy deficit
	F	psia	Btu/hr	Btu/hr		Btu/hr
1	119.535	248	8.18357e+06	87972	0.0734366	8.18357e+06
2	133.599	248.308	7.57413e+06	157914	0.0954015	0
3	148.873	248.615	6.98042e+06	160251	0.118107	0
4	165.835	248.923	6.16405e+06	149725	0.142021	0
5	182.899	249.231	5.02573e+06	128305	0.164806	0
6	199.526	249.538	3.58883e+06	134743	0.185872	0
7	215.045	249.846	2.74412e+06	103405	0.204597	0
8	220.561	250.154	238153	20567	0.211047	0
9	225.716	250.462	380100	20251.9	0.216981	0

Table 4 Profiles / Thermal Analysis.

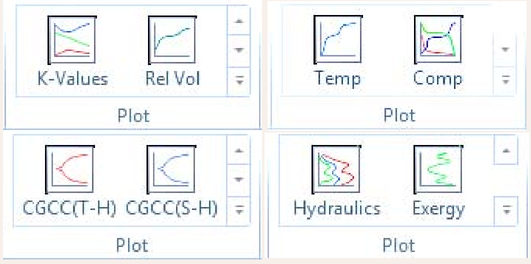


Figure 2 Plot Wizard displays several plots as a part of 'Analysis' and 'Column Targeting Tool.'

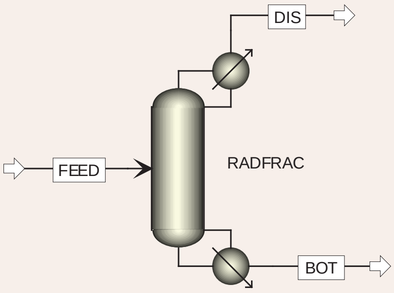


Figure 3 RadFrac column.

Sustainability metrics: potential environmental impact

This study quantifies the sustainability metrics of 'potential environmental impacts,' which is the emissions/unit mass of product and carbon tax**,** by using the Aspen Plus options of (1) 'Carbon Tracking' and (2) 'Global Warming Potential' (GWP).

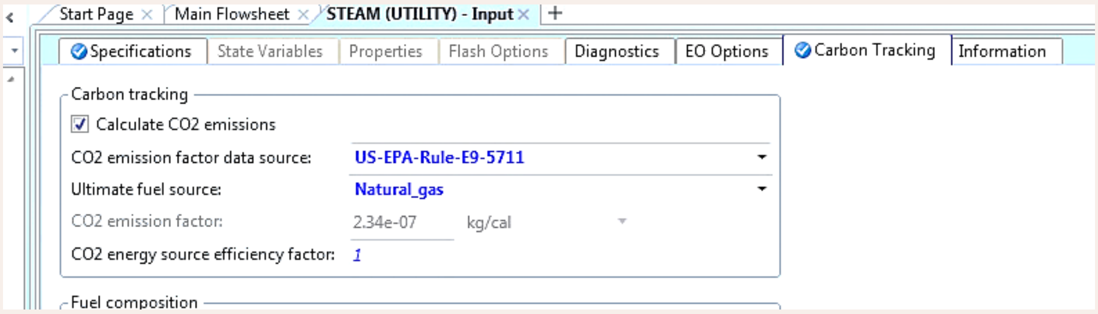
Carbon tracking: In each utility block, 'carbon Tracking' allows the calculation of CO_2 emissions after specifying 'CO_2 emission factor data source' and 'ultimate fuel source' from built-in data. The CO_2 emission factor data source can be from European Commission decision of '2007/589/EC' or United States Environmental Protection Agency Rule of 'E9-5711' [21,22]. This source can also be directly specified by the user. In this example, CO_2 emission factor data source is US-EPA-Rule-E9-5711 and the fuel source is natural gas as seen in (Table 5). The utilities used in the column include cooling water and steam. For example, the steam utility is created as shown in (Table 6). The Results Summary | Operating Costs | Utility Cost Summary sheet displays the total heating and cooling duties as well as their costs (Table 7). The rate and cost of CO_2 emission results would be available within the 'Results Summary / CO_2 Emissions' as seen in (Table 8).

Global warming potential: Aspen Plus reports greenhouse gas emissions in terms of CO_2 equivalents of "Global Warming Potential' (GWP). CO_2 is one of the greenhouse gases that cause around 20% of GWP. To use this feature one can create a property set (Table 9). Prop-Set properties report the carbon equivalents of streams based on data from three popular standards for reporting such emissions: 1) the IPCC's 2nd (SAR), 2) 4th (AR4) Assessment Reports, and 3) the U.S. EPA's (CO_2E-US) proposed rules from 2009 (Table 10) [21,22]. Prop-Set properties are reported in stream reports after selected: Report Options / Streams / Property sets (Table 11). The Setup | Calculation Options | Calculations sheet activates the Standards for 'Global Warming Potential' as well as 'Carbon fee/carbon tax' (Table 12). The 'Results' form of each **'**Utility' block displays the CO_2 equivalents emitted by this utility in each unit operation block where it is used. Each block also reports these CO_2 equivalents in their own results forms together with the other utility results. These results also appear in the report file (Table 13).

Sustainability metrics: energy intensity

This study calculates the sustainability metrics 'Energy intensity' as nonrenewable energy/unit mass of products by using the Aspen plus Column Targeting Tool capabilities of 'Thermal Analysis' and 'Hydraulic Analysis.' Activation of 'Tray Rating' (Table 14) is necessary for the 'Hydraulic Analysis' capabilities

- Column / Tray Rating / New / Setup / Specs
- Column / Analysis / Analysis Options / Hydraulic analysis The CGCCs are helpful in identifying the targets for potential column modifications for



Carbon tracking

☑ Calculate CO2 emissions

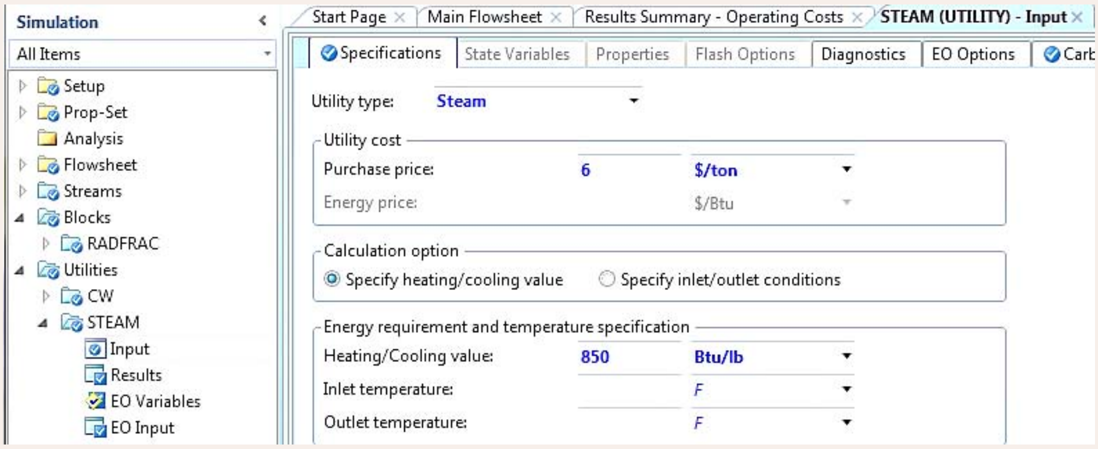
CO2 emission factor data source: US-EPA-Rule-E9-5711

Ultimate fuel source: Natural_gas

CO2 emission factor: 2.34e-07 kg/cal

CO2 energy source efficiency factor: 1

Table 5 Utilities /Steam / Input / Carbon Tracking / Calculate CO2 emissions.



Utility type: Steam

Utility cost

Purchase price: 6 $/ton

Energy price: $/Btu

Calculation option

● Specify heating/cooling value ○ Specify inlet/outlet conditions

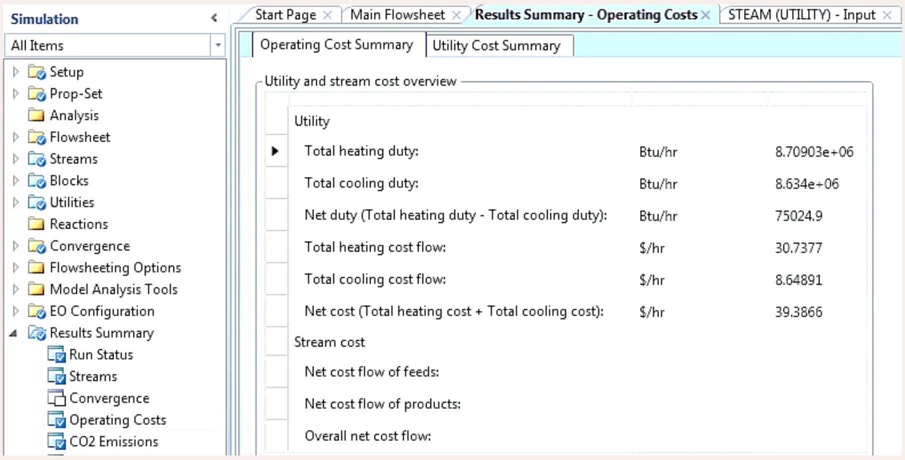
Energy requirement and temperature specification

Heating/Cooling value: 850 Btu/lb

Inlet temperature: F

Outlet temperature: F

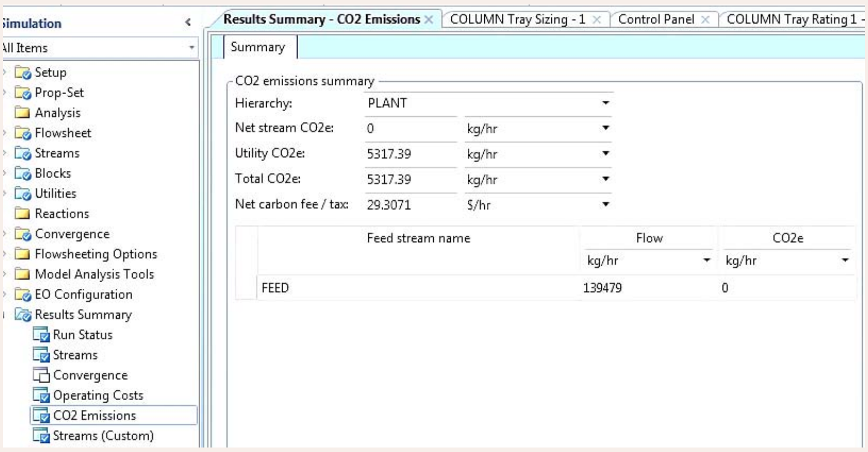
Table 6 Utilities / New / STEAM / Input / Specifications.



Utility and stream cost overview

Utility		
Total heating duty:	Btu/hr	8.70903e+06
Total cooling duty:	Btu/hr	8.634e+06
Net duty (Total heating duty - Total cooling duty):	Btu/hr	75024.9
Total heating cost flow:	$/hr	30.7377
Total cooling cost flow:	$/hr	8.64891
Net cost (Total heating cost + Total cooling cost):	$/hr	39.3866
Stream cost		
Net cost flow of feeds:		
Net cost flow of products:		
Overall net cost flow:		

Table 7 Results Summary | Operating Costs | Operating Cost Summary.

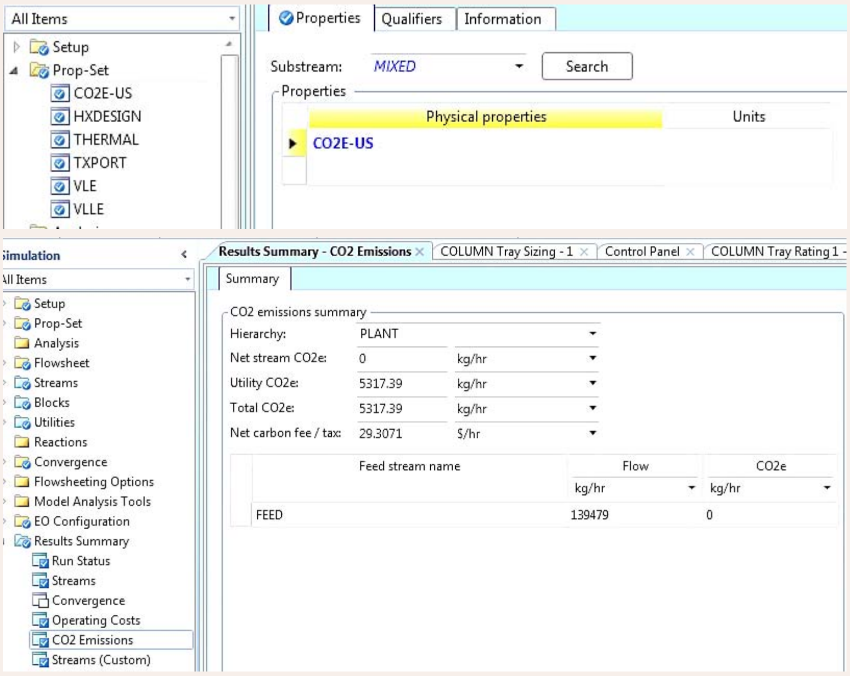


CO2 emissions summary

Hierarchy: PLANT
Net stream CO2e: 0 kg/hr
Utility CO2e: 5317.39 kg/hr
Total CO2e: 5317.39 kg/hr
Net carbon fee / tax: 29.3071 $/hr

Feed stream name	Flow	CO2e
	kg/hr	kg/hr
FEED	139479	0

Table 8 Results Summary / CO2 Emissions / Summary.



Substream: MIXED

Properties

Physical properties	Units
CO2E-US	

CO2 emissions summary

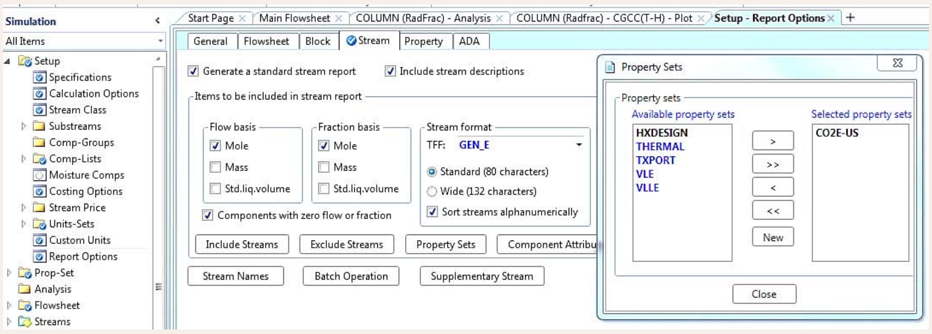
Hierarchy: PLANT
Net stream CO2e: 0 kg/hr
Utility CO2e: 5317.39 kg/hr
Total CO2e: 5317.39 kg/hr
Net carbon fee / tax: 29.3071 $/hr

Feed stream name	Flow	CO2e
	kg/hr	kg/hr
FEED	139479	0

Table 9 Property Set / Properties.

Standards for reporting CO_2 emissions	Prop-Set properties corresponding to each standard
IPCC SAR (1995)	CO2E-SAR
IPCC AR4 (2007)	CO2E-AR4
USEPA (2009)	CO2E-US

Table 10: Standards for reporting CO_2 emissions.



☑ Generate a standard stream report
☑ Include stream descriptions

Items to be included in stream report

Flow basis: ☑ Mole ☐ Mass ☐ Std.liq.volume

Fraction basis: ☑ Mole ☐ Mass ☐ Std.liq.volume

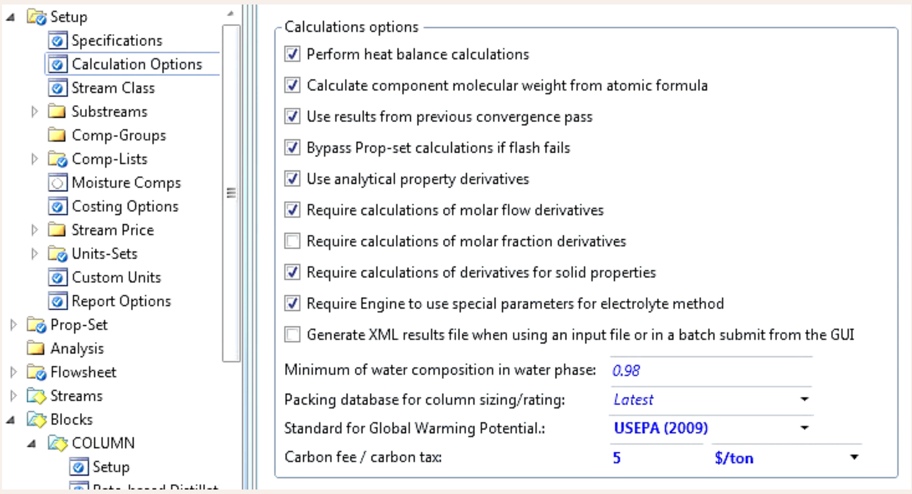
☑ Components with zero flow or fraction

Stream format: TFF: GEN_E
● Standard (80 characters)
○ Wide (132 characters)
☑ Sort streams alphanumerically

Property sets

Available property sets	Selected property sets
HXDESIGN	CO2E-US
THERMAL	
TXPORT	
VLE	
VLLE	

Table 11 Setup | Report Options | Stream / Property Sets.

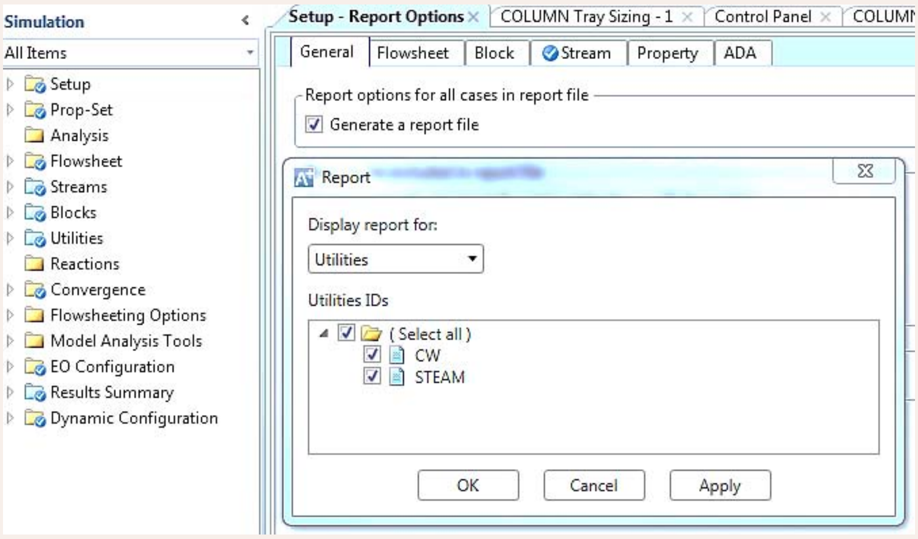


Calculations options

☑ Perform heat balance calculations
☑ Calculate component molecular weight from atomic formula
☑ Use results from previous convergence pass
☑ Bypass Prop-set calculations if flash fails
☑ Use analytical property derivatives
☑ Require calculations of molar flow derivatives
☐ Require calculations of molar fraction derivatives
☑ Require calculations of derivatives for solid properties
☑ Require Engine to use special parameters for electrolyte method
☐ Generate XML results file when using an input file or in a batch submit from the GUI

Minimum of water composition in water phase: 0.98
Packing database for column sizing/rating: Latest
Standard for Global Warming Potential.: USEPA (2009)
Carbon fee / carbon tax: 5 $/ton

Table 12 Setup / Calculation Options / Standard for Global Warming Potential / Carbon fee (tax).



Report options for all cases in report file
☑ Generate a report file

Display report for: Utilities

Utilities IDs
☑ (Select all)
☑ CW
☑ STEAM

Table 13 Report / Utilities.

1. Feed stage location (appropriate placement)
2. Reflux ratio modification (reflux ratio vs. number of stages)
3. Feed conditioning (heating or cooling)
4. Side condensing or reboiling (adding side heater and/or cooler) (Table 15) displays the condenser and reboiler duties as well as the CO_2 emission rate for the base case, while (Table16) shows the carbon fee (tax).

Modifying the feed stage location

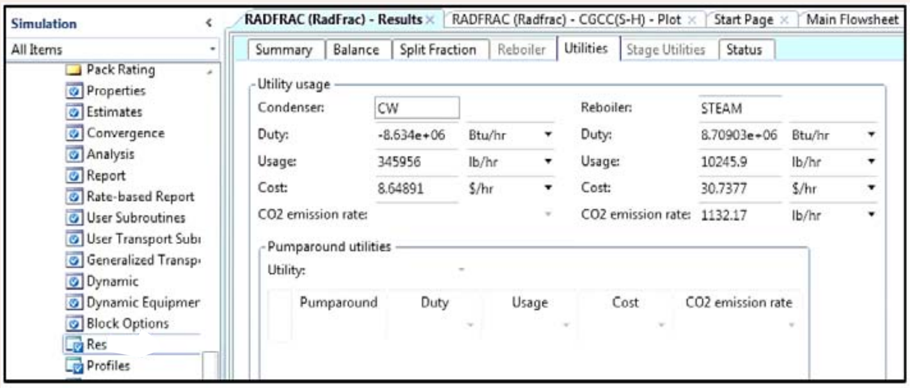
In Aspen Plus, the condenser is the first stage, while the reboiler is the last stage. The Stage-H plots of CGCC can identify distortions because of inappropriate feed placements. The distortions become apparent as significant projections at the feed location called the pinch point due to a need for extra local reflux to compensate for inappropriate feed placement. A correctly introduced feed removes the distortions and reduces the condenser and reboiler duties.

- 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 the column.
- 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 the column [1,20].

For the base operation, Stage-Enthalpy plot displays a sharp change on the condenser side around feed stage 4 (Figure 4). This

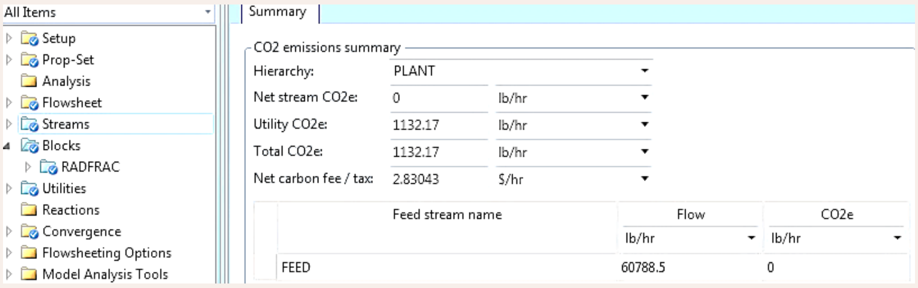
Starting stage: 2
Ending stage: 13
Tray type: Sieve
Number of passes: 1
Diameter: 5.5 ft
Deck thickness: 10 GAUGE
Tray spacing: 2 ft

Table 14 Column / Tray Rating / New / Setup / Specs.



Condenser: CW
Duty: -8.634e+06 Btu/hr
Usage: 345956 lb/hr
Cost: 8.64891 $/hr
CO2 emission rate:
Reboiler: STEAM
Duty: 8.70903e+06 Btu/hr
Usage: 10245.9 lb/hr
Cost: 30.7377 $/hr
CO2 emission rate: 1132.17 lb/hr

Table 15 Base case: NF = 4; RadFrac / Results : CO2 emission rate = 1132.2 lb/hr.



Hierarchy: PLANT
Net stream CO2e: 0 lb/hr
Utility CO2e: 1132.17 lb/hr
Total CO2e: 1132.17 lb/hr
Net carbon fee / tax: 2.83043 $/hr

Feed stream name	Flow	CO2e
	lb/hr	lb/hr
FEED	60788.5	0

Table 16 Base case: Result Summary / CO2 Emissions: Net carbon fee = $2.83/hr.

should be corrected by moving the feed stage down.

Condenser side projects excessive loss of accessible work: Ex_{loss} = 300,000 Btu/hr (Figure 5). This may be due to misplaced feed location and original partial condenser load and column configuration. The 'Hydraulic Analysis' is activated after creating the 'Tray Rating.' Hydraulic Analysis display three important flow plots: ideal minimum flow, actual flow, and hydraulic maximum flow, the plots indicate that between stages 1 to 4 actual and ideal flows are far apart from each other (Figure 6). Moving the feed stage from 4 to 7 removes the sharp changes around the feed stage 4 as seen in (Figure 7). The sustainability metrics after moving the feed stage from 4 to 7 show the reduction of

- CO_2 emission rate from 1132.2 lb/hr to 1077.4 lb/hr representing a 4.8% decrease as seen in (Tables 16 and Table 17).
- Condenser duty from -8.634e+6 Btu/hr to -8.183e+6 Btu/hr.
- Reboiler duty from 8.714e+6 Btu/hr to 8.28e+6 Btu/hr.
- The net carbon fee decreased from \$2.8/hr to \$2.7/hr (Tables 16 and Table 18).
- Table 19 indicates that other alternative feed stages 6 would not produce favorable CO_2 emission rate; the rate of 1084.6 lb/hr for NF = 6 is higher than that of 1077.4 lb/hr for NF = 7. Hence it is disregarded.

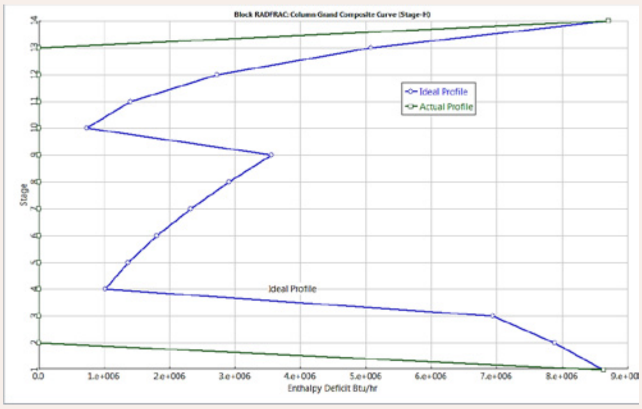


Figure 4 Base case: NF=4; Stage-Enthalpy plot of Column Grand Composite Curve.

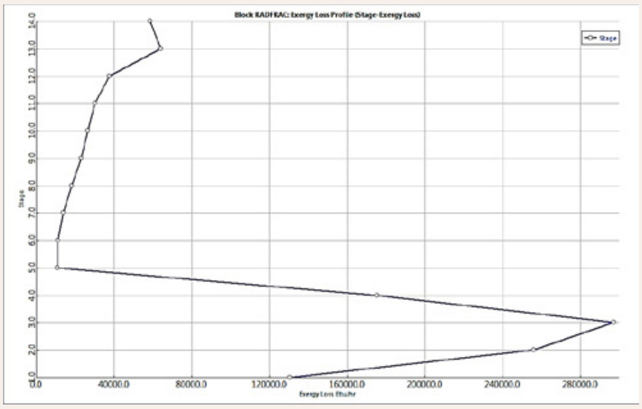


Figure 5 Base case: NF = 4: Analysis / Exergy loss profile.

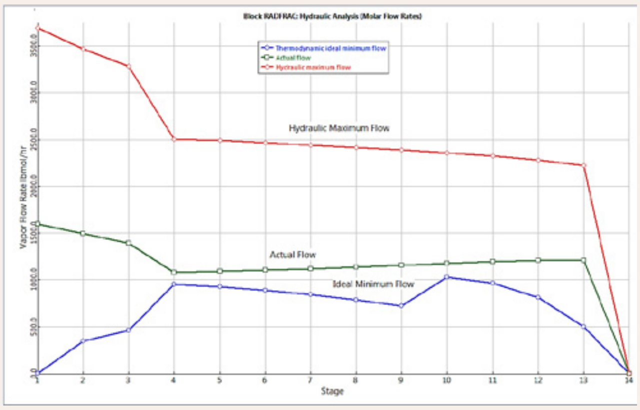


Figure 6 Base case: NF = 4; Analysis / Hydraulic Analysis.

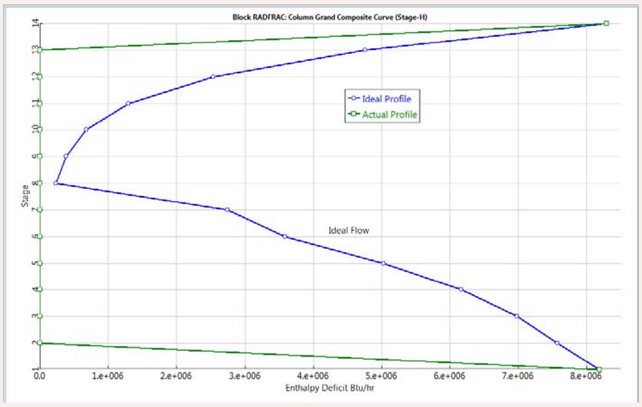
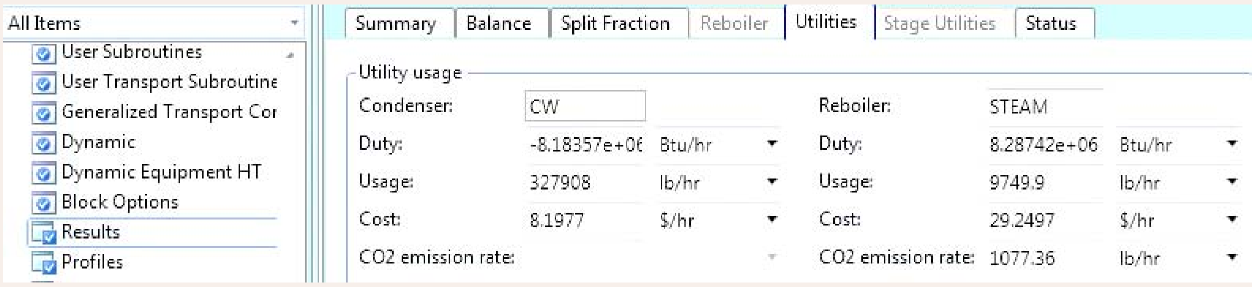


Figure 7 Modified case I: NF = 7; Analysis / Stage-Enthalpy.

Figure 8 Modified case I: NF = 7; Analysis / Stage-Exergy Loss Profile. Ex_{loss} = 160,000 Btu/hr.

Figures 5 and Figure 8 indicate that the maximum rate of exergy loss is reduced from 300,000 Btu/hr to 160,000 Btu/hr after moving the feed stage from 4 to 7.This represents around 46% reduction in the accessible work loss after the modification.

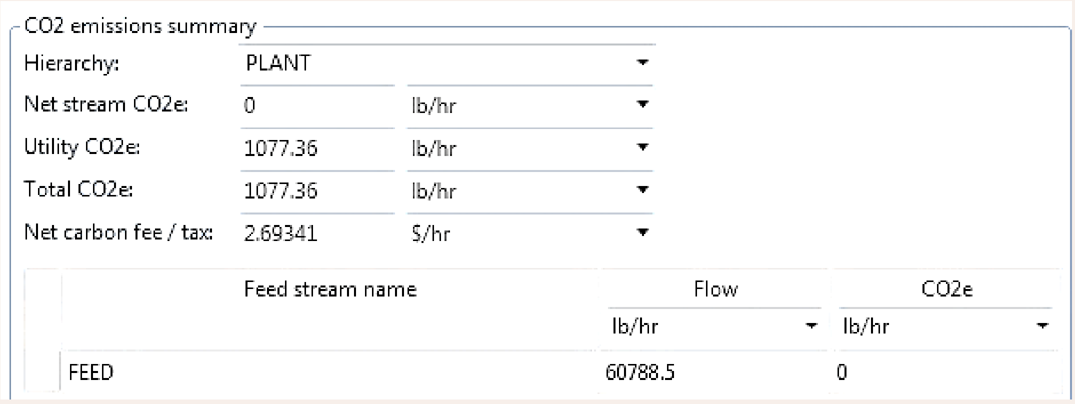
Modifying the reflux ratio



Utility usage

Condenser:	CW		Reboiler:	STEAM	
Duty:	-8.18357e+06	Btu/hr	Duty:	8.28742e+06	Btu/hr
Usage:	327908	lb/hr	Usage:	9749.9	lb/hr
Cost:	8.1977	$/hr	Cost:	29.2497	$/hr
CO2 emission rate:			CO2 emission rate:	1077.36	lb/hr

Table 17 Modified case I: NF = 7; RADFRAC / Results / Utilities.

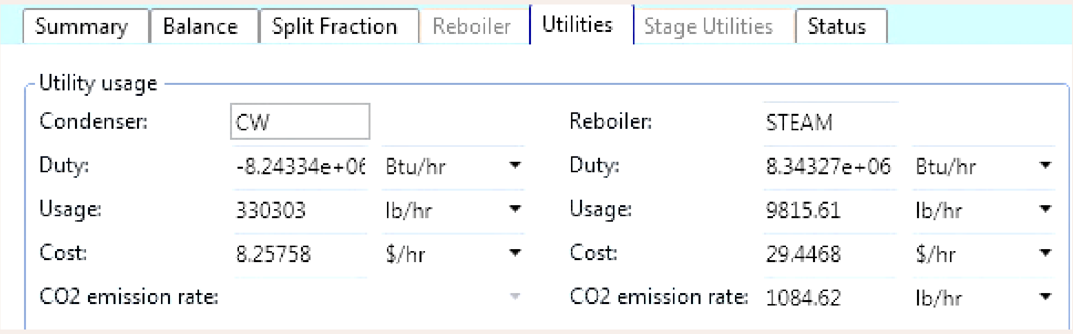


CO2 emissions summary

Hierarchy:	PLANT	
Net stream CO2e:	0	lb/hr
Utility CO2e:	1077.36	lb/hr
Total CO2e:	1077.36	lb/hr
Net carbon fee / tax:	2.69341	$/hr

Feed stream name	Flow	CO2e
	lb/hr	lb/hr
FEED	60788.5	0

Table 18 Modified case I: NF = 7; Result summary / CO2 Emissions / Summary.



Utility usage

Condenser:	CW		Reboiler:	STEAM	
Duty:	-8.24334e+06	Btu/hr	Duty:	8.34327e+06	Btu/hr
Usage:	330303	lb/hr	Usage:	9815.61	lb/hr
Cost:	8.25758	$/hr	Cost:	29.4468	$/hr
CO2 emission rate:			CO2 emission rate:	1084.62	lb/hr

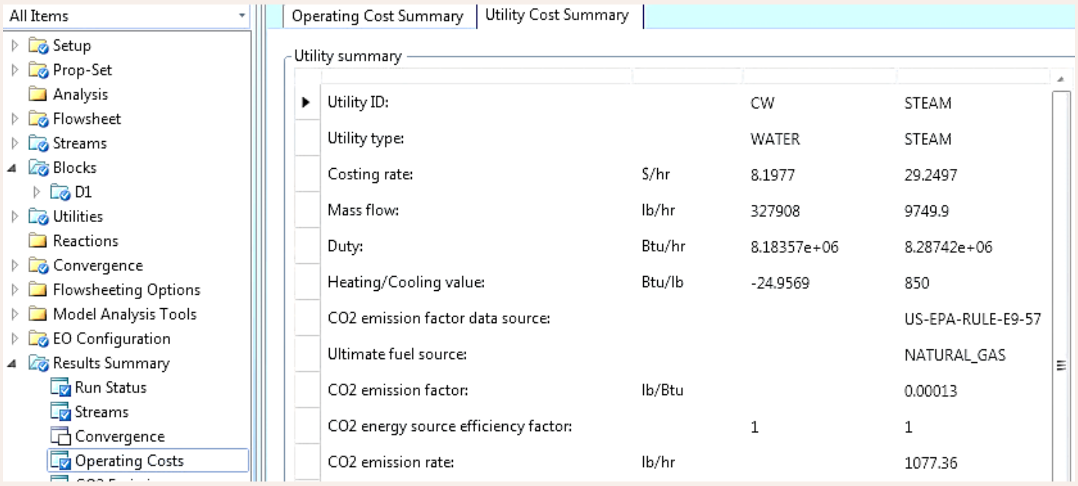
Table 19 Modified case II: NF = 6; Results / Utilities.

The horizontal gap between the CGGC T-H pinch point and the ordinate represents the excess heat, and therefore, the scope for a reduction in reflux ratio [7,18]. As the reflux ratio is reduced the CGCC will move towards the ordinate and hence reduce both the reboiler and condenser duties. However, to preserve the separation, the number of stages must increase. Figure 7 and Table 20 with the modified feed stage and will represent the base case for possible reflux ratio (RR= 6.06) modifications: 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. In the first modification, reflux ratio is reduced to RR = 4.5 from RR = 6.06. As the reflux ratio is reduced, number of stages is increased to N = 20 with the feed stage NF = 12 (instead of NF = 7). Figure 9 displays the CGCC Stage-H plot. Table 21 indicates that with the decreased reflux ratio from 6.06 to 4.5

- CO_2 emission rate decreased from 1077.4 lb/hr to 813.1 lb/hr (around 24% reduction in CO_2 emission).
- The reboiler duty decreased from 8.28 e+06 Btu/hr to 6.25 e+06 Btu/hr, which caused the reduction in CO_2 emission.
- The condenser duty decreased from 8.19 e+06 Btu/hr to 6.16 e+06 Btu/hr.

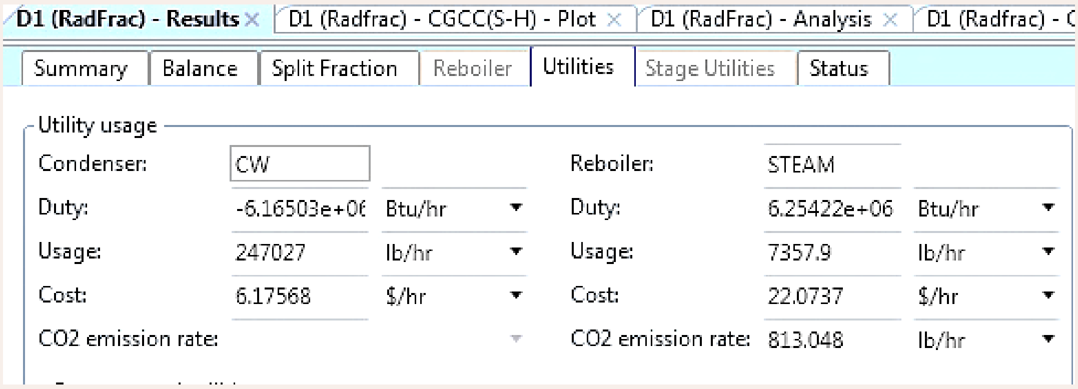
In the second modification, (Figure 10) shows the CGCC with RR = 2.5, N = 28 and NF = 14. As (Table 22) indicates that with the decreased reflux ratio from 6.06 to 2.5

- CO_2 emission rate decreased from 1077.4 lb/hr to 479.8 lb/hr (around 55% reduction)
- The reboiler duty decreased from 8.28e+06 Btu/hr to 3.69e+06 Btu/hr.
- The condenser duty decreased from 8.19 e+06 Btu/hr to



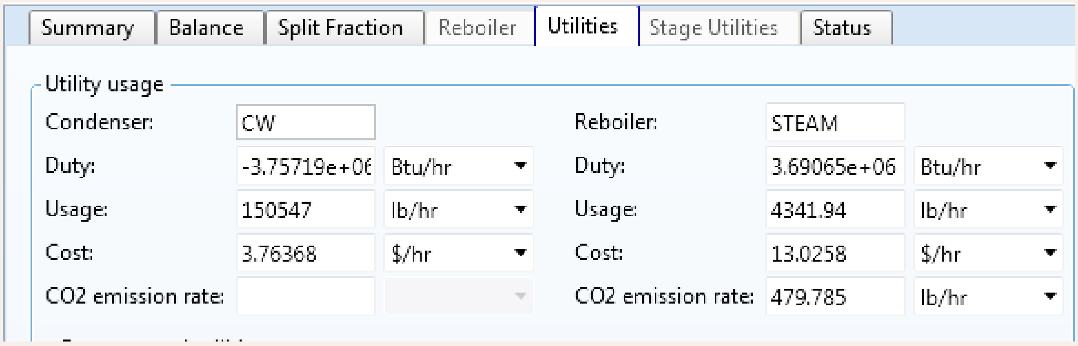
Utility ID:		CW	STEAM
Utility type:		WATER	STEAM
Costing rate:	$/hr	8.1977	29.2497
Mass flow:	lb/hr	327908	9749.9
Duty:	Btu/hr	8.18357e+06	8.28742e+06
Heating/Cooling value:	Btu/lb	-24.9569	850
CO2 emission factor data source:			US-EPA-RULE-E9-57
Ultimate fuel source:			NATURAL_GAS
CO2 emission factor:	lb/Btu		0.00013
CO2 energy source efficiency factor:		1	1
CO2 emission rate:	lb/hr		1077.36

Table 20 Base Case I: N = 14, NF=7; RR= 6.06; Results Summary / Operating Costs.



Condenser:	CW		Reboiler:	STEAM	
Duty:	-6.16503e+0	Btu/hr	Duty:	6.25422e+06	Btu/hr
Usage:	247027	lb/hr	Usage:	7357.9	lb/hr
Cost:	6.17568	$/hr	Cost:	22.0737	$/hr
CO2 emission rate:			CO2 emission rate:	813.048	lb/hr

Table 21 Modified case I: N = 20, NF=12; RR= 4.5.



Condenser:	CW		Reboiler:	STEAM	
Duty:	-3.75719e+0	Btu/hr	Duty:	3.69065e+06	Btu/hr
Usage:	150547	lb/hr	Usage:	4341.94	lb/hr
Cost:	3.76368	$/hr	Cost:	13.0258	$/hr
CO2 emission rate:			CO2 emission rate:	479.785	lb/hr

Table 22 Modified case II: N = 28, NF=14; RR= 2.5; Results / Utilities.

3.75e+06 Btu/hr.

- Net carbon fee is reduced from $2.7/hr to $1.2/hr, as seen in (Table 23).

With the decreased reflux ratio from 6.06 to 2.5, (Figure 11) indicates that

- The exergy loss at the condenser is reduced from Ex_{loss} = 160000 Btu/hr to Ex_{loss} = 55,000 Btu/hr.
- The exergy loss at the feed stage is reduced from Ex_{loss} = 135000 Btu/hr to Ex_{loss} = 30,000 Btu/hr.

As seen in (Figure 12), except the stages close to condenser, the actual flow closely follows the thermodynamic ideal minimum flow with the decreased reflux ratio from 6.06 to 2.5. This represents close to optimum flow conditions in most of the stages.

Feed conditioning

Figure 7 and Figure 8, and (Table 17) display the base case with the feed temperature of 225°F. The need for an adjustment of feed quality can be identified from sharp enthalpy changes on the stage-H or temperature-H CGCC plot

- If a feed is excessively sub-cooled, the T-H CGCC plots will 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 T-H CGCC plots will 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 will lead to similar duty changes in the column reboiler or condenser loads, respectively.

There is a sharp change in enthalpy above the feed stage yet it is not close to reboiler in the CGCC Stage-Enthalpy plot shown in (Figure 7). This still indicates sub cooling of the feed; therefore, feed temperature should be increased. In the modification, the feed temperature is increased from 225°F to 250°F. Figure 13 shows the S-H CGCC. Table 24 shows that after preheating

- The reboiler duty decreased from Q_R = 8.3e+06 Btu/hr to Q_R = 4.3e+06 B tu/hr and the cost decreased from $29/hr to $15/hr.
- The condenser duty increased from Q_C = 8.18e+06 Btu/hr to Q_C = 8.80e+06 B tu/hr and the cost decreased from $8.2/hr to $8.8/hr.
- The CO_2 emission decreased from 1077 lb/hr to 555.8 lb/hr.

Figure 14 shows that the exergy loss increased from 160000 Btu/hr to 230000 Btu/hr around the condenser due to the increased cooling duty.

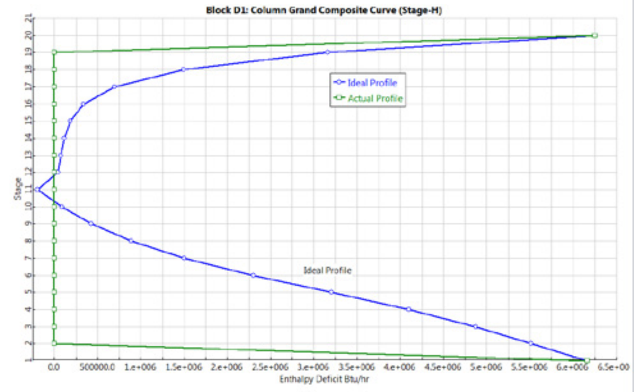


Figure 9 Modified case I: N = 20, NF=12; RR= 4.5; Analysis / CGCC Stage Enthalpy.

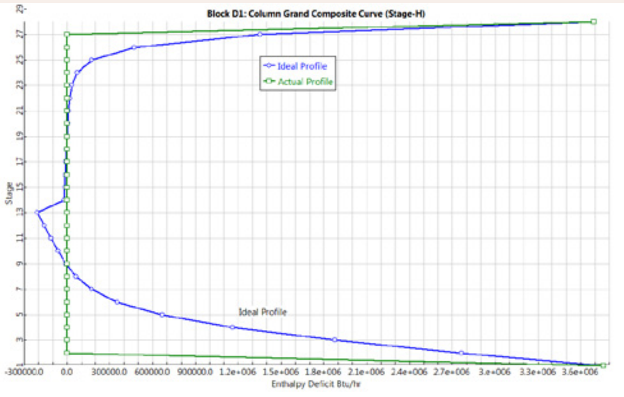


Figure 10 Modified case II: N = 28, NF=14; RR= 2.5; Analysis / CGCC Stage-Enthalpy.

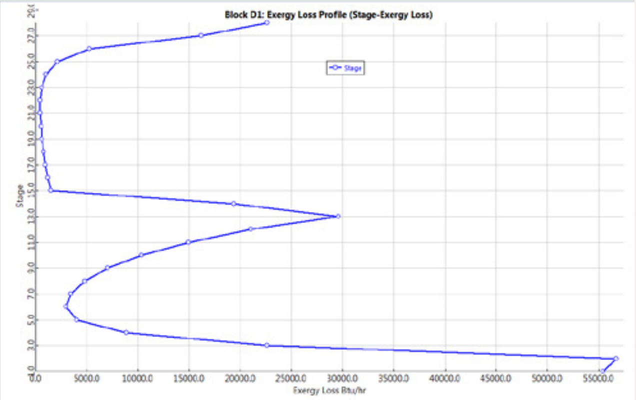


Figure 11 Modified case II: N = 28, NF=14; RR= 2.5; Analysis / Stage-Exergy loss.

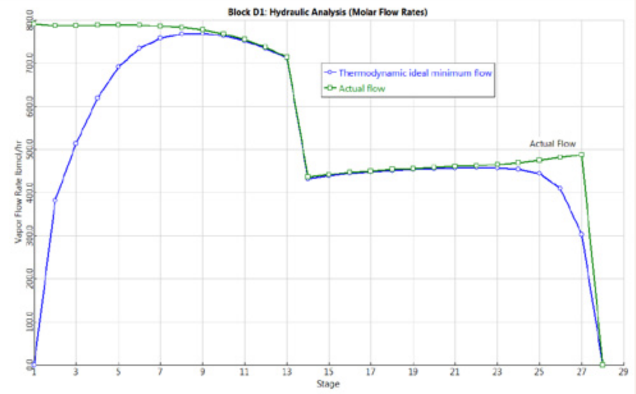


Figure 12 Modified case II: N = 28, NF=14; RR= 2.5; Analysis / Hydraulic Analysis.

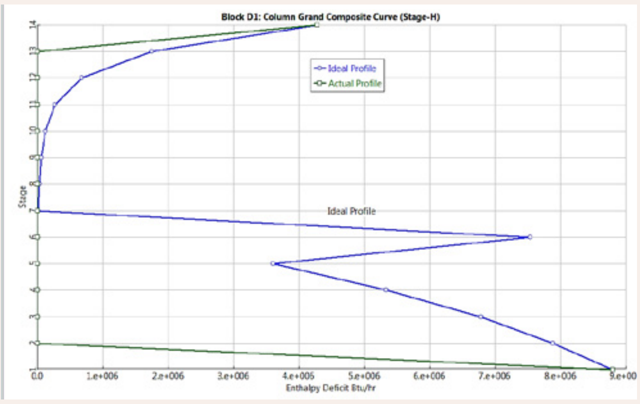
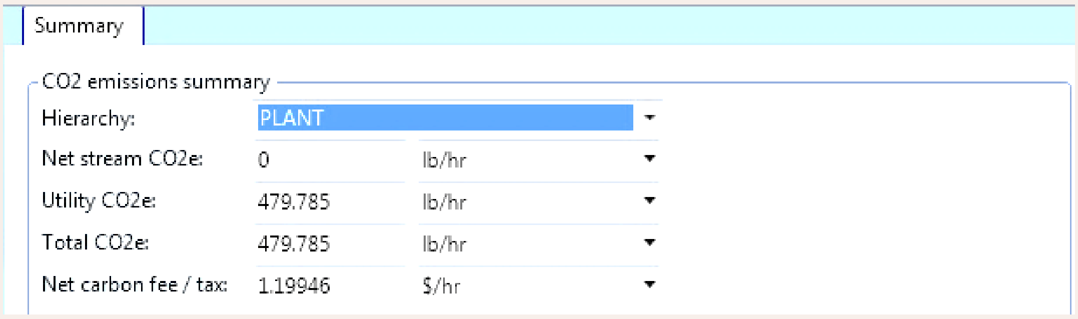


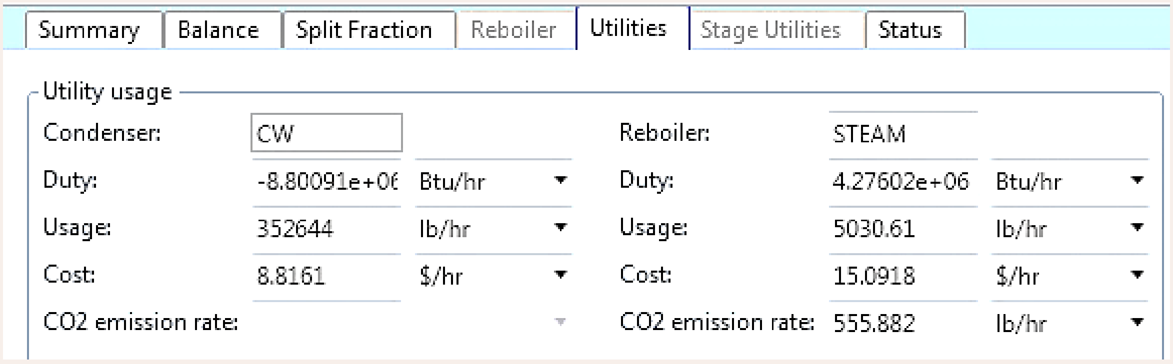
Figure 13 Modified case I: TF =250 oF; RR=6.05; N = 14; NF = 7; Analysis / Thermal Analysis CGCC Stage-Enthalpy.



CO2 emissions summary

Hierarchy:	PLANT	
Net stream CO2e:	0	lb/hr
Utility CO2e:	479.785	lb/hr
Total CO2e:	479.785	lb/hr
Net carbon fee / tax:	1.19946	$/hr

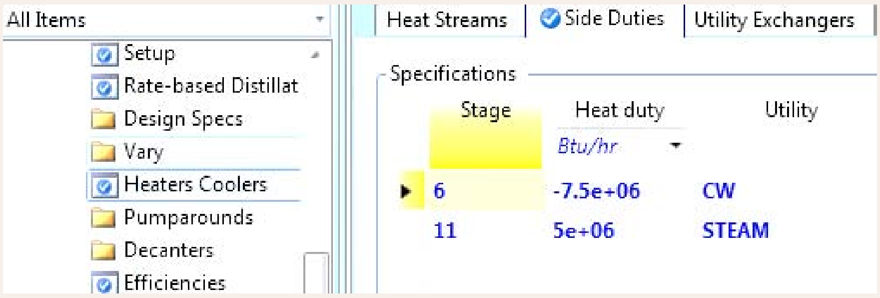
Table 23 Results Summary / CO2 Emissions / Net carbon fee.



Utility usage

Condenser:	CW		Reboiler:	STEAM	
Duty:	-8.80091e+06	Btu/hr	Duty:	4.27602e+06	Btu/hr
Usage:	352644	lb/hr	Usage:	5030.61	lb/hr
Cost:	8.8161	$/hr	Cost:	15.0918	$/hr
CO2 emission rate:			CO2 emission rate:	555.882	lb/hr

Table 24 Results/ Utilities.



Specifications

Stage	Heat duty Btu/hr	Utility
6	-7.5e+06	CW
11	5e+06	STEAM

Table 25 Side heater installation: Heaters Coolers / Side Duties.

Side condensing or side reboiling

Feed conditioning is usually preferred to side condensing or side reboiling. Side condensing or side reboiling is external modification at a convenient temperature level. The scope for side condensing or side reboiling can be identified from the area beneath and/or above the CGCC pinch point (area between the ideal and actual enthalpy profiles). This area could be reduced by integrating side condensing and/or reboiling on an appropriate stage [1,19,10,18]. 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, hence 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, hence lowering the overall operating costs.

Table 17 and Figure 7 represent the base case. Figure 7

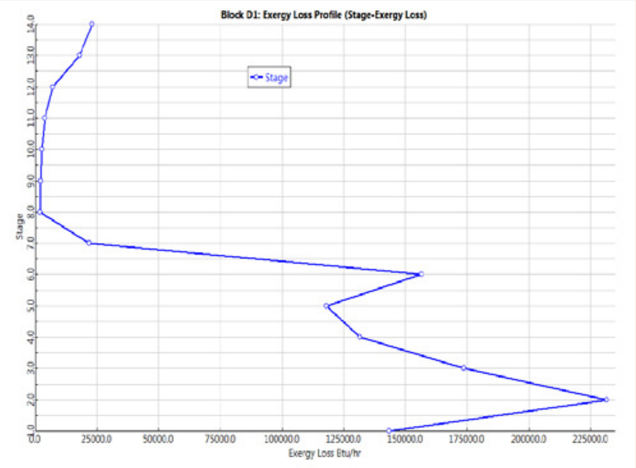


Figure 14 Modified case I: TF =250 oF; RR=6.05; N = 14; NF = 7; Analysis / Thermal Analysis CGCC Stage-Exergy loss.

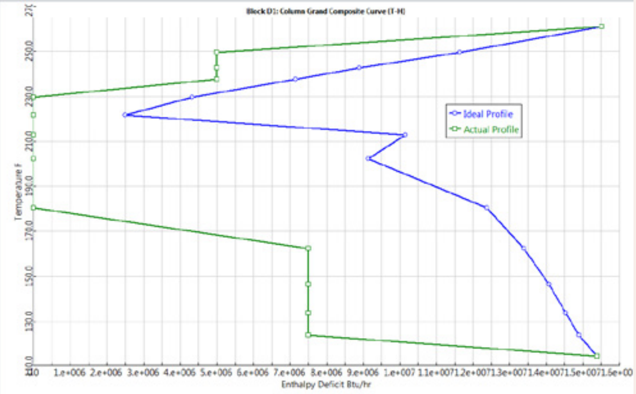


Figure 15 Modified case: TF =225 oF; RR=6.05; N = 14; NF = 7; Analysis / Thermal Analysis / CGCC Temperature-Enthalpy; Side cooler at stage 6: QC = −7.5e+06; Side heater at stage 11: Q_R = 5e+06.

shows a significant area existing below and above the pinch between ideal and actual profiles; therefore a side condenser and a heater can be placed at convenient temperature levels (stages). In this modification, a side condenser is installed at stage 6 to remove −7.5e+06 Btu/hr and a side heater is installed at stage 11 supplying 5.0e+06 Btu/hr at a cheaper rate. Side condensers and heaters are installed using '**Heaters Coolers'** block (Table 25) (Figure 15) displays the CGCC temperature-enthalpy plot.

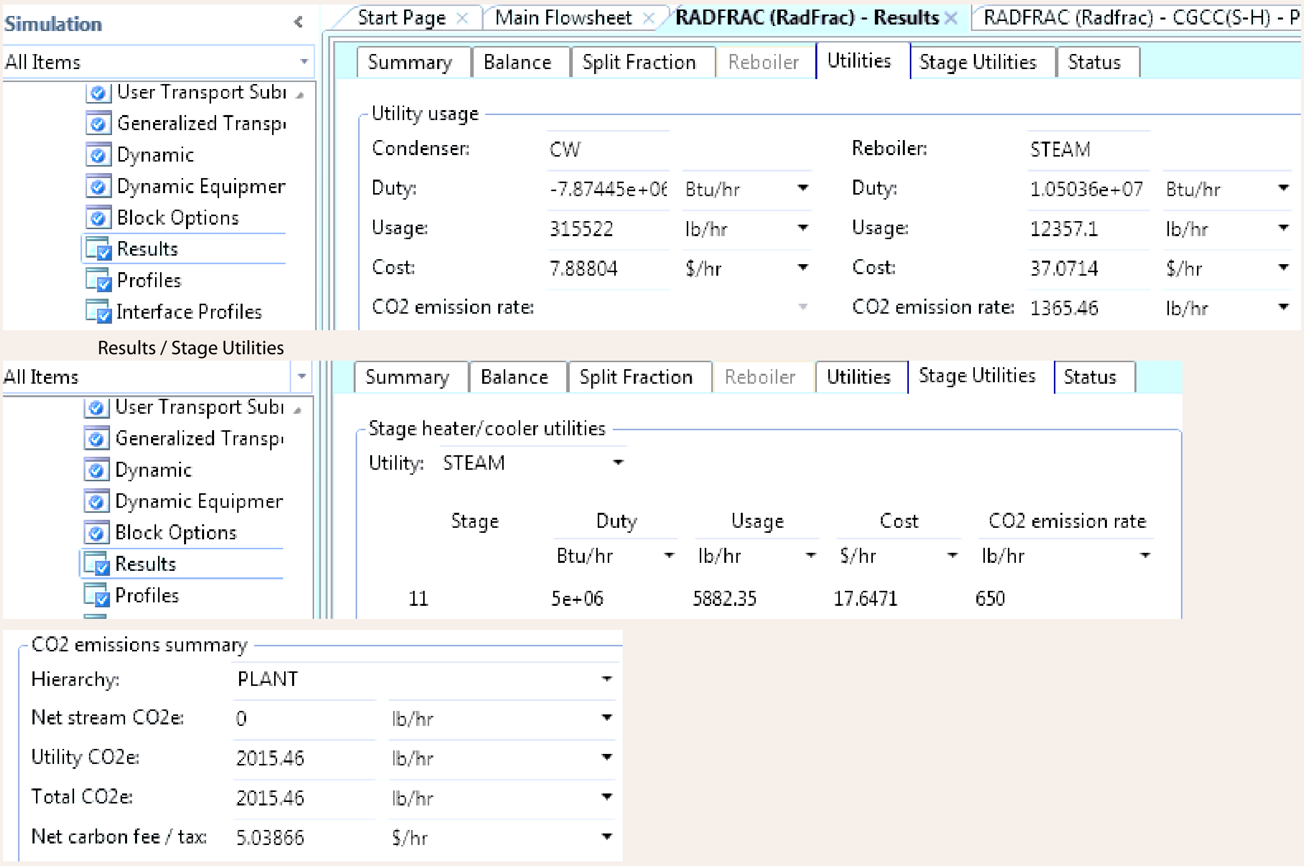
Tables 4, 26 shows that

- Total condenser duty increased to (−7.874e+06 -7.5e+06) Btu/hr from −8,2e+06 Btu/hr.
- Total reboiler duty increased to (−1.050e+07 +5.0e+06) Btu/hr from 8,28e+06 Btu/hr.
- CO_2 emission rate increased to 2015 lb/hr from 1077 lb/hr.

Table 26 shows the increase in energy usage, CO_2 emission, and net carbon fee. Also, the cost of external installation of heat exchangers has to be considered. Overall these modifications do not lead to sustainable operation as they violate the both sustainable metrics of 'Energy intensity' and 'Potential environmental impact.'

CONCLUSIONS

This study demonstrates a conceptual design tool of the Aspen Plus simulator for sustainable operation of distillation columns, which are highly energy intensive and an important part of chemical and petrochemical process industries. The 'Column Targeting Tool (CTT)' can help reduce the use of energy and hence CO_2 emission. The 'Carbon Tracking (CT)' and 'Global Warming Potential' options can help quantify the reduction in CO_2 emission. They can be part of sustainability metrics of 'Energy intensity' and 'Potential environmental impact' for existing and new design of distillation column operations. An integrated approach of combination of column targeting tools, carbon tracking, pinch analysis with existing process heats, and



Utility usage

Condenser:	CW		Reboiler:	STEAM	
Duty:	-7.87445e+06	Btu/hr	Duty:	1.05036e+07	Btu/hr
Usage:	315522	lb/hr	Usage:	12357.1	lb/hr
Cost:	7.88804	$/hr	Cost:	37.0714	$/hr
CO2 emission rate:			CO2 emission rate:	1365.46	lb/hr

Results / Stage Utilities

Stage heater/cooler utilities

Utility: STEAM

Stage	Duty	Usage	Cost	CO2 emission rate
	Btu/hr	lb/hr	$/hr	lb/hr
11	5e+06	5882.35	17.6471	650

CO2 emissions summary

Hierarchy:	PLANT	
Net stream CO2e:	0	lb/hr
Utility CO2e:	2015.46	lb/hr
Total CO2e:	2015.46	lb/hr
Net carbon fee / tax:	5.03866	$/hr

Table 26 Modified case: TF =225 oF; RR=6.05; N = 14; NF = 7; Results / Utilities; Side cooler at stage 6: Q_C = −7.5e+06 Btu/hr; Side heater at stage 11: Q_R = 5e+06 Btu/hr.

overall process simulation may lead to sustainable chemical and petrochemical process industries.

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Cite this article

Demirel Y (2013) Sustainable Operations for Distillation Columns. Chem Eng Process Tech 1: 1005.