

Exergy analysis of a Top Heat-Integrated Distillation Columns (T-HIDiC) for Propylene-Propane system

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Abstract

Exergy analysis by Grassmann Diagram of a Top heat-integrated distillation column (T-HIDiC), is conducted and compared against conventional and vapor recompression columns, for the system propylene-propane. In addition, within the T-HIDiC, three different operational conditions are compared: 1) T-HIDiC with equilibrium stages, 2) T-HIDiC with tray efficiency and 3) T-HIDiC in equilibrium but not heat-integrated. The analysis showed by thermodynamical consideration that the T-HIDiC has high potential for exergy loss reduction compared with conventional and vapor recompression columns in equilibrium conditions, reducing exergy losses in 61.2% and 14.5%, respectively. It was also demonstrated the great effect that occurs on the exergy losses when considering the efficiency of the plate in the T-HIDiC, reaching an increase of the losses almost 6 times for the case study with the efficiencies worked. The exergy benefit of implementing heat integration was observed when comparing T-HIDiC with and without energy integration, achieving a reduction of around 3.5 times in exergy losses when performing heat integration.

Keywords: T-HIDiC; Distillation; Exergy; Grassmann diagram, Heat transfer; Propylene, Propane.

1. Introduction

Distillation columns are major energy consumers in the chemical and petrochemical industries (Gorak & Sorensen, 2014). Conventional distillation columns tend to have low second law efficiencies. An important condition that reduces the column efficiency is the way heat load is distributed through the column (Mendoza & Riascos, 2011). In order to reduce energy consumption, considerable studies have been carried out and many distillation columns have been proposed. The Heat-Integrated Distillation Column (HIDiC) is a non-conventional distillation column developed from the diabatic distillation concept (M. Nakaiwa et al., 2003; M Nakaiwa et al., 1997). A HIDiC (Fig. 1a) is constructed to provide the driving forces for heat transfer from the rectifying to the stripping sections, the former must be operated at a higher pressure than the latter.

Detailed descriptions of HIDiC technology and some implementations are presented elsewhere (Kiss & Olujic, 2014). The energy savings, compared to conventional columns, estimated by several authors (Liu & Qian, 2000; Matsuda et al., 2010; M Nakaiwa et al., 1997; Masaru Nakaiwa et al., 2001) are from 52 to 90%, these studies considered systems with relative volatilities from 1.15 (propylene-propane) to 2.40 (benzene-toluene). Within the concentric type HIDiC there are several configurations, see Fig. 1b. However, within all these settings, for the Propylene-propane study system, the configuration that presented the best results, based on exergy loss, is the Top-HIDiC (Mancera et al., 2018). For this reason, the exergy analysis by Grassmann diagram was carried out on this configuration and was compared with the conventional column, the vapor recompression column (VRC), T-HIDiC with plate efficiency and T-HIDiC without heat integration.

Exergy can be defined as the useful work potential of the system at the specified state to the state of its environment (Boles & Yunus A. Cengel, 2014; Kotas, 1995). The exergy of a substance can generally be divided into two parts: Thermo-mechanical exergy (physical, heat and work), and chemical exergy (mixing/separation and reaction) (Delmar, 2019).

In this work, we limit the study to thermo-mechanical exergy, in special to the exergy transfer by mass, heat and work, and thus disregard any chemical exergy present.

1.1. Physical exergy (exergy transfer by mass)

Physical exergy is a function of enthalpy and entropy differences measured between an initial and final state (Delmar, 2019):

$$Ex = H(T, P) - H_0(T_0, P_0) - T_0[S(T, P) - S_0(T_0, P_0)] \quad (eq. 1)$$

This is the equation for the calculation of physical exergy where Ex is the exergy flow, H is the enthalpy, S is entropy, P is pressure, T is the starting temperature while H_0 , T_0 , P_0 and S_0 refer to those values at environmental or reference conditions.

1.2. Exergy Transfer by Heat

Heat is a form of disorganized energy, and thus only a portion of it can be converted to work, which is a form of organized energy (the second law). Therefore, heat transfer is always accompanied by exergy transfer. Heat transfer Q at a location at thermodynamic temperature T is always accompanied by exergy transfer in the amount of (Kotas, 1995):

$$Ex_{heat} = Q(1 - T_0/T) \quad (eq. 2)$$

where Q is the heat produced or used.

1.3. Exergy Transfer by Work

Exergy is defined as the maximum work potential so that the exergy in a process is the same as the work available from that process where work is represented by W .

$$Ex_{work} = W \quad (eq. 3)$$

1.4. Exergy loss

The exergy destroyed is proportional to the entropy generated and they are related to each other by the Gouy-Stodola theorem (de Koeijer & Rivero, 2003):

$$Ex^{loss} = T_0 dS^{irr}/dT \quad (eq. 4)$$

By dividing the exergy loss by the reference temperature ($T_0 = 298,15$ K), the corresponding entropy production rate of the exergy benchmark is obtained.

A more general calculation of the exergy loss, in steady state, can be carried out by using the exergy balance, as described below:

$$Ex^{loss} = Ex_{in} - Ex_{out} \quad (eq. 5)$$

Where Ex_{in} and Ex_{out} are the entering and leaving total rates of exergy respectively, transferred by heat, work, and mass.

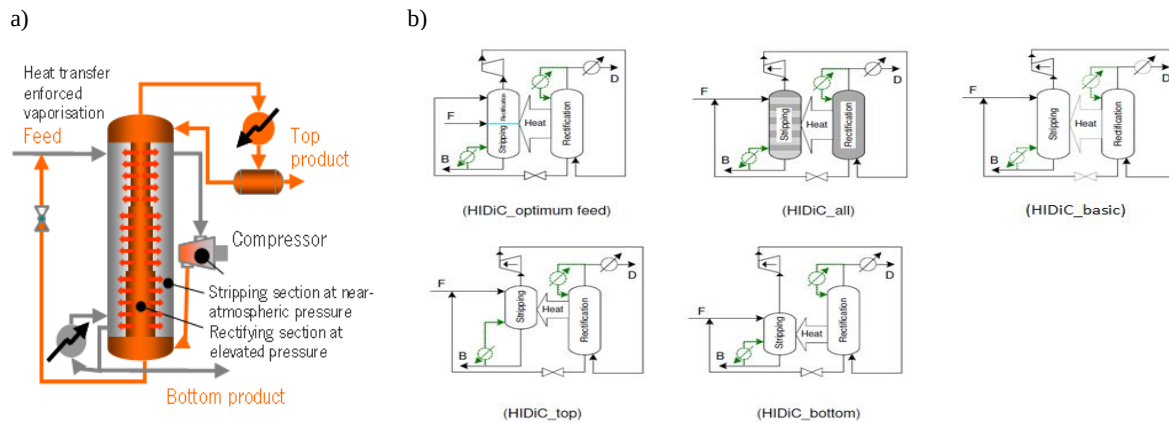


Figure 1: a) Concentric HIDiC scheme. (Source: Process Systems Enterprise) b) Configuration options schematic for concentric HIDiC columns (Pulido, 2008)

1.5. Grassmann Diagram

This type of diagram is a graphical representation similar to the well-known Sankey diagram employed in the energy analysis of processes, where the width of the bands is associated to the exergy rate or exergy flow rate (Grassmann, 1959; Oliveira, 2013). Its advantage lies in quickly showing, visually, the inflow and outflow amounts of exergy, as well as the exergy losses in each equipment of the process that is being studied (de Koeijer & Rivero, 2003).

2. Methodology

To perform the exergy analysis, two types of simulations were carried out:

- 1) Simulation taking into account the type of column. To carry out this part, three simulations were run, each with a different type of column: a) Conventional Column, b) Vapor Recompression Column (VRC) and c) Top Heat-Integrated Distillation Column (T-HIDiC in equilibrium). The objective in this step is to compare the three column types and to validate the exergy advantage of using the T-HIDiC column.
- 2) Simulation with three different types of T-HIDiC configuration: a) T-HIDiC in equilibrium, b) T-HIDiC with tray efficiency and c) T-HIDiC without heat integration. (This simulation is carried out solely to corroborate the exergy benefit of energy integration). The objective in this step is to quantify the effect of the inclusion of the plate efficiency on the exergy and possible benefits of heat integration on the exergy losses.

The conditions used for the simulations are based in the work of Mancera et al., (2018), taking the conditions of the Top-HIDiC column because it was the configuration that presented the best results for the studied system (Propylene-Propane). Columns were simulated in Aspen Plus 8.1 using Peng-Robinson equation of state (EOS) model to calculate thermodynamic properties, including vapor-liquid equilibrium. The simulations were carried out in steady state, using isentropic efficiency in the compressor (VRC and Top-HIDiC), and heat flow does not occur between system and surroundings. The conditions are shown in Table 1.

Table 1: Parameters and set up for process simulation using Aspen plus

Characteristic	Conventional	VRC	T-HIDiC equilibrium	T-HIDiC efficiency	T-HIDiC without heat integrated
Rectification section Pressure(bar)	11,2	11,2	14,6	14,6	14,6
Stripping section pressure (bar)	11,2	11,2	11,2	11,2	11,2
Stages rectification section	164	164	170	170	170
Stages stripping section	47	47	61	61	61
Feeding stage	165	165	171	171	171
Trays in the Concentric Column	---	--	169	169	169
Trays in the Annular column	---	--	60	60	60
Feed flow (kg / h)	112000	112000	112000	112000	112000
Fraction mol food (propylene)	0,57	0,57	0,57	0,57	0,57
Thermal condition food (q)	0,37	0,37	0,37	0,37	0,37
Murphree efficiency stripping	---	---	---	47,02% *	---
Murphree efficiency rectification	---	---	---	49,5% *	---
Fraction mol distillate (propylene)	0,996	0,996	0,996	0,996	0,996
Fraction mol funds (propylene)	0,011	0,011	0,011	0,011	0,011
Compressor (isentropic) efficiency	---	0,72	0,72	0,72	0,72

* The efficiency data are taken from previous work of the authors obtained by CFD simulation for a perforated plate of a column T-HIDiC.

The scheme selected for the heat distribution between the rectification section and the stripping section for the Top-HIDiC was the uniform heat transfer area using the procedure suggested by Suphanit (2010), Fig. 2. After specifying the components and thermodynamic model, the column configuration is simulated as shown in Fig. 3c.

2.1 Exergy calculation

The exergy calculation was performed for each of the streams involved in each of the equipment that is part of the distillation process, according to equations 1, 2 and 3. The reference conditions or dead state are temperature of 298,15K and pressure of 1 atm. This calculation was carried out for each of the configurations mentioned above.

For the calculation of the exergy loss in each piece of equipment, Equation 5 was used. Next, the specific equations corresponding to the exergy loss for each of the equipment are written according to the type of column.

2.1.1 Exergy loss calculations for the conventional column

The equations used to calculate the exergy losses in each equipment of the conventional distillation system are described below (see Fig. 3a):

Reboiler:

$$Ex_{Reb}^{loss,C1} = A_{steam}^{C1}(Ex_{steam,in}^{C1} - Ex_{steam,out}^{C1}) + L_{210}^{C1}Ex_{L210}^{C1} - V_{211}^{C1}Ex_{V211}^{C1} - B^{C1}Ex_B \quad (eq. 6)$$

Column:

$$Ex_{Col}^{loss,C1} = F_{Feed}^{C1}Ex_{feed}^{C1} + R^{C1}Ex_{Reflux}^{C1} + V_{211}^{C1}Ex_{V211}^{C1} - V_2^{C1}Ex_{V2}^{C1} - L_{210}^{C1}Ex_{L210}^{C1} \quad (eq. 7)$$

Condenser:

$$Ex_{cond}^{loss,C1} = A_{watercool}^{C1}(Ex_{watercool,in}^{C1} - Ex_{watercool,out}^{C1}) + V_2^{C1}Ex_{V2}^{C1} - L_1^{C1}Ex_{L1}^{C1} \quad (eq. 8)$$

Where,

$$L_1^{C1} = R^{C1} + Dist^{C1} \quad (eq. 9)$$

The superscript C1, in equations 6 – 9 is placed to specify that it is the conventional column. A_{steam} , $A_{watercool}$, R , F_{feed} , B and $Dist$ are heating steam, cooling water, reflux, feed, bottom and distillation flows respectively. V_i and L_i are vapor and liquid flows in i th stage.

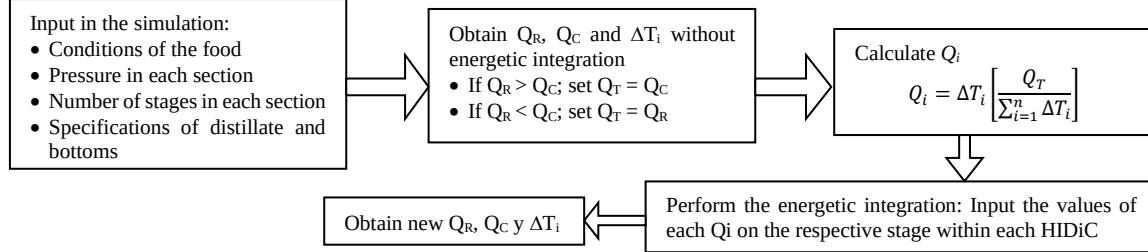


Figure 2: Procedure for the Heat distribution between the rectification section and the stripping section

2.1.2 Exergy loss calculations for the vapor recompression column

The equations used to calculate the exergy losses in each equipment of the vapor recompression distillation system are described below (see Fig. 3b):

Reboiler:

$$Ex_{Reb}^{loss,C2} = V_{comp}^{C2}Ex_{Vcomp}^{C2} + L_{210}^{C2}Ex_{L210}^{C2} - V_{211}^{C2}Ex_{V211}^{C2} - L_{val,in}^{C2}Ex_{Lval,in}^{C2} - B^{C2}Ex_B^{C2} \quad (eq. 10)$$

Column:

$$Ex_{Col}^{loss,C2} = F_{Feed}^{C2}Ex_{feed}^{C2} + R^{C2}Ex_{Reflux}^{C2} + V_{211}^{C2}Ex_{V211}^{C2} - V_2^{C2}Ex_{V2}^{C2} - L_{210}^{C2}Ex_{L210}^{C2} \quad (eq. 11)$$

Compressor:

$$Ex_{Comp}^{loss,C2} = V_2^{C2}Ex_{V2}^{C2} + W_{comp}^{C2} - V_{comp}^{C2}Ex_{Vcomp}^{C2} \quad (eq. 12)$$

Valve:

$$Ex_{Valv}^{loss,C2} = L_{val,in}^{C2}Ex_{Lval,in}^{C2} + L_{val,out}^{C2}Ex_{Lval,out}^{C2} \quad (eq. 13)$$

Condenser:

$$Ex_{cond}^{loss,C2} = A_{watercool}^{C2}(Ex_{watercool,in}^{C2} - Ex_{watercool,out}^{C2}) + L_{val,out}^{C2}Ex_{Lval,out}^{C2} - L_1^{C2}Ex_{L1}^{C2} \quad (eq. 14)$$

where

$$L_1^{C2} = R^{C2} + Dist^{C2} \quad (eq. 15)$$

The superscript C2, in equations 10 – 15 is placed to specify that it is the vapor recompression column.

2.1.3 Exergy loss calculations for the T-HiDiC

The equations used to calculate the exergy losses in each unit of the T-HiDiC distillation system are described below (see Fig. 3c):

Reboiler:

$$Ex_{Reb}^{loss,C3} = A_{steam}^{C3}(Ex_{steam,in}^{C3} - Ex_{steam,out}^{C3}) + L_{60,S}^{C3}Ex_{L60,S}^{C3} - V_{61,S}^{C3}Ex_{V61,S}^{C3} - B^{C3}Ex_B^{C3} \quad (eq. 16)$$

Stripping Column:

$$Ex_{Strip}^{loss,C3} = F_{Feed}^{C3}Ex_{feed}^{C3} + L_{val,out}^{C3}Ex_{Lval,out}^{C3} + Ex_{QStrip} + V_{61,S}^{C3}Ex_{V61,S}^{C3} - V_{1,S}^{C3}Ex_{V1,S}^{C3} - L_{60,S}^{C3}Ex_{L60,S}^{C3} \quad (eq. 17)$$

In where Ex_{QStrip} is the exergy due to the energy integration effect given by the heat transfer from the rectification column to the stripping column.

$$Ex_{QStrip} = \sum_{n=1}^{60} Q_n \left(1 - \frac{T_0}{T_n^S} \right) \quad (eq. 18)$$

Compressor:

$$Ex_{Comp}^{loss,C3} = V_{1,S}^{C3}Ex_{V1,S}^{C3} + W_{comp}^{C3} - V_{170,R}^{C3}Ex_{V170,R}^{C3} \quad (eq. 19)$$

Rectification Column:

$$Ex_{Rect}^{loss,C3} = R^{C3}Ex_{Reflux}^{C3} + V_{170,R}^{C3}Ex_{V170,R}^{C3} - Ex_{QRect} - V_{2,R}^{C3}Ex_{V2,R}^{C3} - L_{val,in}^{C3}Ex_{Lval,in}^{C3} \quad (eq. 20)$$

In where Ex_{QRect} is the exergy due to the energy integration effect given by the heat transfer from the rectification column to the stripping column.

$$Ex_{QRect} = \sum_{n=2}^{61} Q_n \left(1 - \frac{T_0}{T_n^R} \right) \quad (eq. 21)$$

Valve:

$$Ex_{Valv}^{loss,C3} = L_{val,in}^{C3}Ex_{Lval,in}^{C3} + L_{val,out}^{C3}Ex_{Lval,out}^{C3} \quad (eq. 22)$$

Condenser:

$$Ex_{cond}^{loss,C3} = A_{watercool}^{C3}(Ex_{watercool,in}^{C3} - Ex_{watercool,out}^{C3}) + V_{2,R}^{C3}Ex_{V2,R}^{C3} - L_{1,R}^{C3}Ex_{L1,R}^{C3} \quad (eq. 23)$$

where

$$L_{1,R}^{C3} = R^{C3} + Dist^{C3} \quad (eq. 24)$$

For the case T-HiDiC without heat integration, the equations 18 and 21 are equal to zero. The superscript C3, in equations 16 – 24 is placed to specify that it is the T-HiDiC.

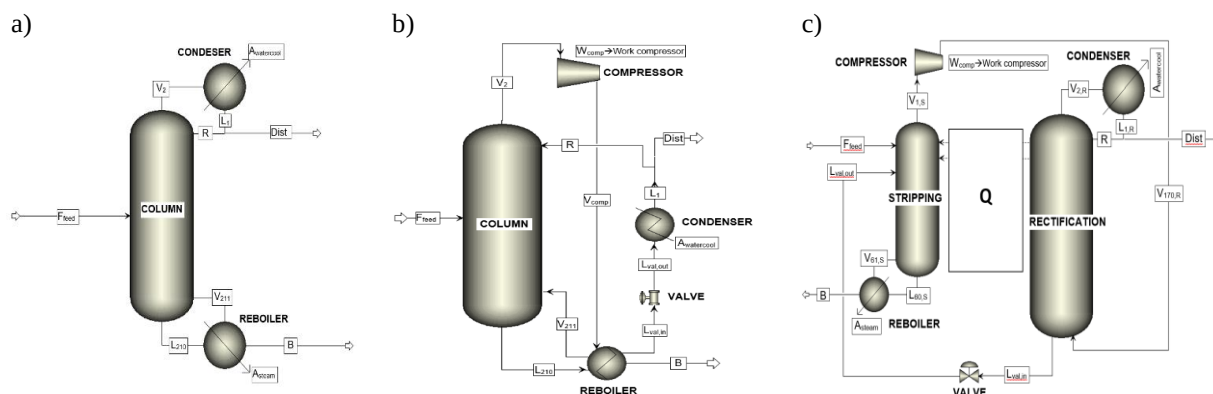


Figure 3: Flow diagram to exergy calculation of a) conventional column, b) VCR and c) T-HiDiC

Once the exergy values were obtained, the Sankey flow show software was used to make the Grassmann diagram. This software can be obtained from the website www.sankeyflows.com in different versions.

3. Results and discussion

Retaking what was raised as the objective of the paper and the cases that were studied, now, the results obtained in the development of the work are presented.

3.1 Simulation results taking into account the type of column.

The exergy flows considering the type of column are shown in Fig. 4. In these diagrams the blue rectangles indicate the equipment that are part of the process, the arrows entering each of these pieces of equipment are the input exergy and the arrows pointing outward are the exergy flows of each labeled stream and the exergy losses generated in each equipment. Each arrow shows the amount, in GJ/hr, of its respective exergy flow. From Fig. 4a it can be determined that the total exergy loss for the conventional column is 68,27 GJ/h, with the boiler being the main cause of this loss, followed by condenser and then the column, as shown in the Table 2 (column 2). In the case of the VRC, the total exergy loss is 30.96 GJ/hr (Fig. 4b). The percentage of participation of each piece of equipment is shown in Table 2 (column 3), with the reboiler being the equipment that contributes the biggest loss, with a percentage of 42.2. Regarding the T-HiDiC in equilibrium, Fig. 4c, it is achieved that the total exergy loss is 26.47 GJ/hr and, in the same way as the previous ones, the percentage of participation of each equipment in this loss, is shown in Table 2 (column 4). Again, the reboiler contributes to the greatest loss with 36.2%.

Table 2: Percentage of exergy loss per equipment in conventional column, VRC and T-HiDiC

Equipment	% exergy loss of each equipment		
	Conventional	VRC	T-HiDiC
Reboiler	91.8	42.2	36.2
Compressor	---	24.6	18.1
Condenser	4.2	2.5	16.0
Rectification	---	---	14.8
Stripping	---	---	10.3
Valve	---	8.4	4.6
Column	4.0	22.3	---

From the total exergy loss data, once again it is verified that of the three types of columns, the one that generates the lowest exergy losses is the T-HiDiC as shown in Table 3. This table also shows the percentages of reduction of exergy losses of the VRC and T-HiDiC column concerning the conventional column, as well as the percentage of reduction of the exergy loss of T-HiDiC concerning the VRC.

Table 3: Exergy loss and percentage of reduction per column

Column	Exergy loss (GJ/hr)	% reduction in exergy loss compared to the conventional column	% reduction in exergy loss compared to the VRC
Conventional	68.27	---	---
VRC	30.96	54.65	---
T-HiDiC equil.	26.47	61.22	14.49

It is also important to mention, in general terms, that for the three types of columns, it is observed that the internal exergy flows are much greater than the input and output exergy flows, for example, in the conventional column the reflux is 104.78 GJ/hr compared to an exergy flow of the distillate and the feed stream of 7.71 GJ/hr and 14.20 GJ/hr, respectively. This is due to the high reflux ratio that is handled as a consequence of the propylene-propane system having a relative volatility close to one.

3.2 Simulation results with three different types of T-HiDiC configuration

The results are presented, using Grassmann diagrams, of the configurations established in the methodology for the T-HiDiC, as shown in Fig. 5. For the case of the equilibrium T-HiDiC, the result is given in Fig. 4c.

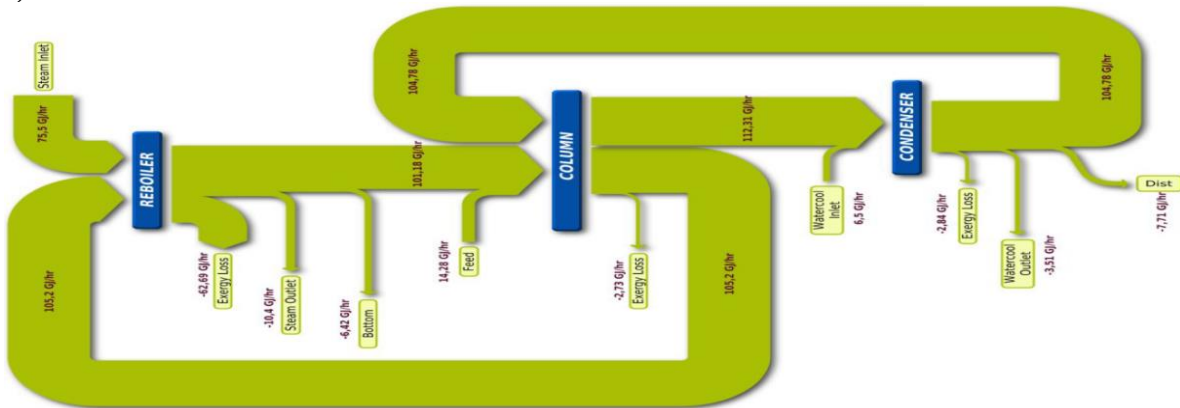
From Fig. 5a, it is determined that the total exergy loss for T-HiDiC with tray efficiency is 157.77 GJ/hr. The percentage of participation of each piece of equipment in this loss is discriminated, as shown in Table 4 (column 2), being the reboiler, the equipment that contributes to the largest loss with a percentage of 63.6%, well above the others.

Table 4: Exergy loss per equipment in T-HiDiC with tray efficiency and without heat integration

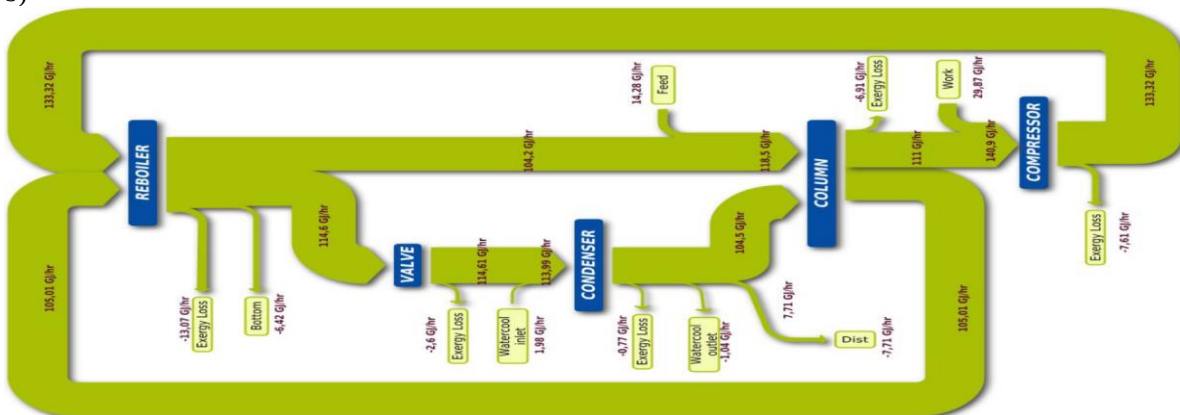
Equipment	% exergy loss	
	T-HiDiC with tray efficiency	T-HiDiC without heat integration
Reboiler	63.6	68.1
Condenser	17.9	18.9
Compressor	6.7	4.5
Rectification	5.4	2.8
Stripping	4.6	4.5
Valve	1.8	1.2

For the case of the T-HIDiC without heat integration between the rectification and stripping columns, from Fig. 5b it is obtained that the total exergy loss is 93.4 GJ/hr, where the percentage of participation of each equipment is shown in Table 4 (column 3), with the reboiler being the equipment that contributes to the greatest loss with a percentage of 68.1%.

a)



b)



c)

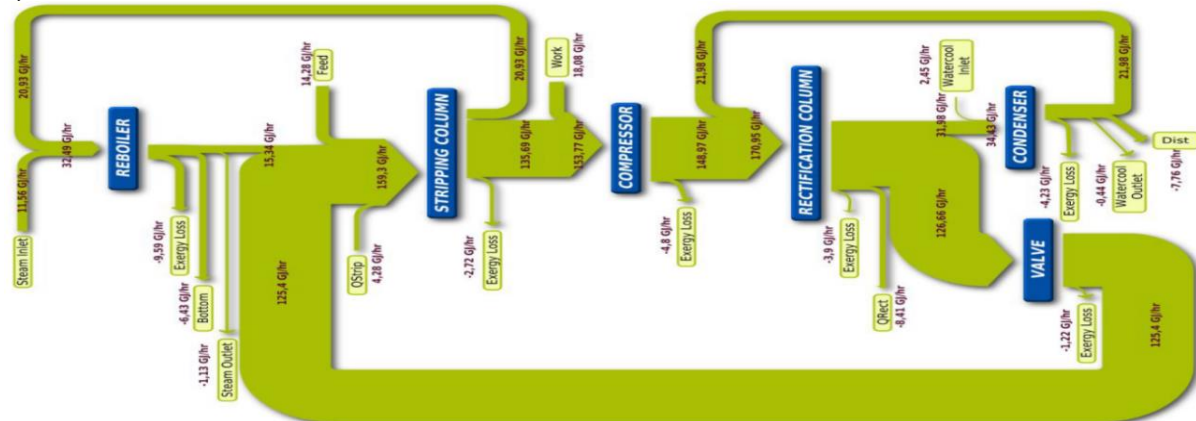


Figure 4: Grassmann Diagram of a) Conventional column, b) VRC and c) T-HIDiC in equilibrium

The exergy losses are compared between the three configurations in Table 5. It is observed that the inclusion of the efficiency in the column, as expected, increases the exergy losses, however this increase is almost 6 times more compared to the T-HIDiC in equilibrium, for the efficiencies worked, showing that the effect of the efficiency on the exergy losses is not linear in nature but rather exhibits an exponential behavior, since decreasing the efficiency close to half (around 48%), losses increased 6 times from 26.7 to 157.77 GJ/hr. Regarding the T-HIDiC without heat integration compared to the HIDiC in equilibrium, its increase in exergy losses was around 3.5 times more, showing once again the benefits of energy integration over exergy losses.

Table 5: Exergy loss and percentage of reduction per column for different configurations of T-HIDiC

Column	Exergy loss (GJ/hr)	% reduction in exergy losses compared to T-HIDiC with efficiency	% reduction in exergy losses compared to T-HIDiC without integration
T-HIDiC efficiency	157.77	---	----
T-HIDiC without integration	93.4	40.79	----
T-HIDiC equil.	26.47	83.22	71.66

It is also interesting to note that both the T-HIDiC with try efficiency and the T-HIDiC without integration give greater losses of exergy than the conventional column and the VRC, however, it should be mentioned that the latter two are in equilibrium condition, therefore in order to make a more equitable comparison of the T-HIDiC with efficiency with respect to the conventional column and VRC, the simulations of these columns would have to be carried out with the efficiency criterion included.

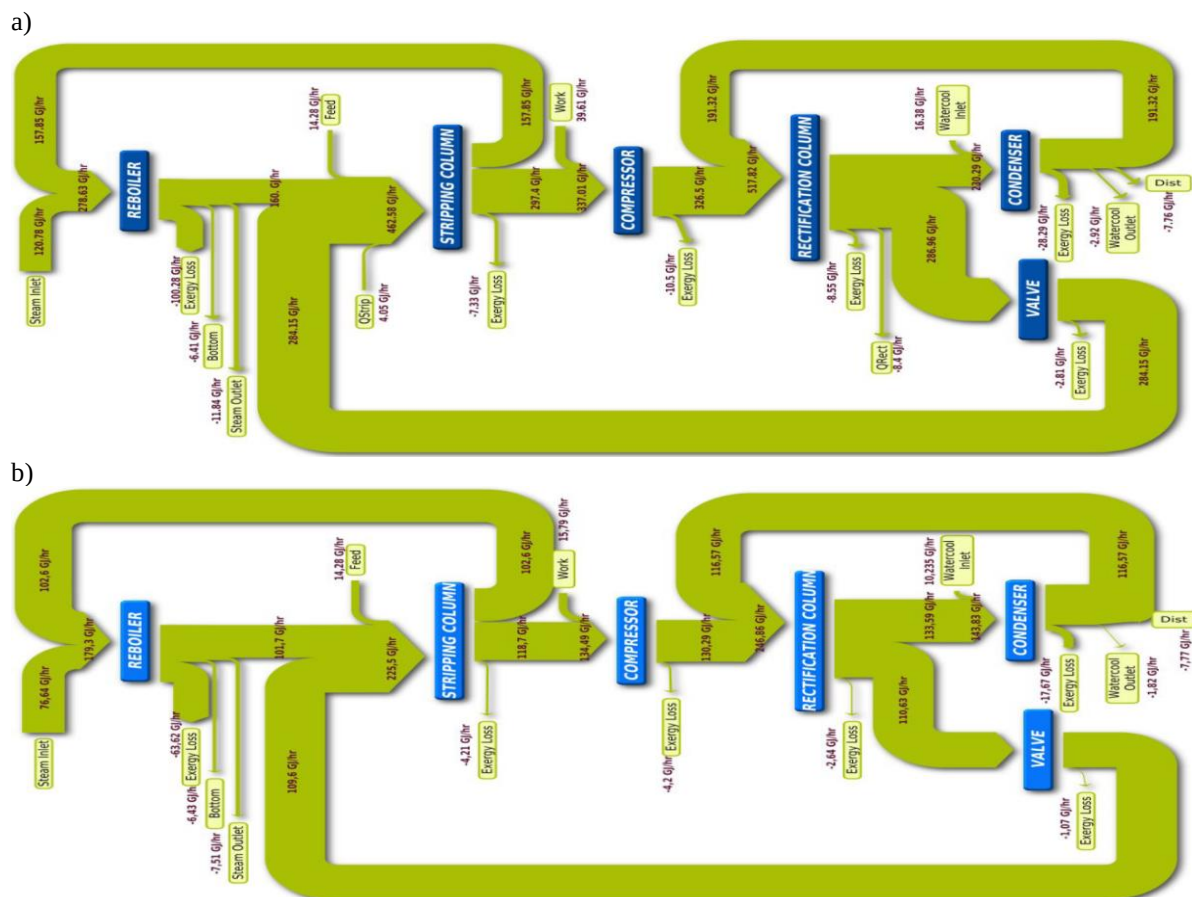


Figure 5: Grassmann Diagram of a) T-HIDiC with efficiency tray and b) T-HIDiC without heat integrated. Regarding the T-HIDiC without integration, although it gives greater losses than the conventional column and the VRC, it does not justify the direct comparison with these columns, since this simulation is carried out as an exercise to demonstrate the benefit of integration, since the purpose of building a HIDiC, regardless of its configuration, is the heat integration.

4. Conclusions

The reduction of the exergy loss of the T-HIDiC in equilibrium with respect to the conventional column and the VRC is 54,65% and 14,49% respectively.

By applying an efficiency of 47% for the rectification section and 49% for the stripping section, in T-HIDiC, the exergy losses increase about 6 times more with respect to equilibrium, becoming even less effective than the conventional column and the VRC in equilibrium. However, for a better comparison, it is recommended to perform the exergy analysis for the conventional column and the VRC column, each working with efficiencies.

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