

Applying Exergy Analysis for Simulation and Optimization of the Iso-butane Recovery Process from Liquefied Petroleum Gas

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This paper presents the analysis of several distillation process configurations for the recovery of iso-butane from a mixture of iso-butane and n-butane from liquefied petroleum gas (LPG), which is produced at Dinh Co GPP in Ba Ria Vung Tau – Vietnam. This project uses the method of process simulations followed by exergy and cost analysis in order to compare the efficiency of energy utilization among the process configuration options. Simulation of a base case and two other distillation process configuration options for separating iso-butane from LPG are implemented via Aspen HYSYS software using Peng-Robinson EOS (equation of state). Exergy is a thermodynamic concept based on the first and second laws to identify process configuration options that use energy inefficiently by locating and quantifying energy wasted through irreversibility or exergy lost. For a base case, the conventional distillation column is simulated with the specified iso-butane product drawn as the side stream. The other process configuration options are a direct sequence distillation and a dividing wall column distillation. The simulation results of the columns are recorded with the purity specifications of about 95 % of mass iso-butane in product streams and the recovery ratio of iso-butane exceeding 95 %. Then exergy analysis is conducted for each of the three distillation process configurations to find the process configuration in the scope of most efficient energy usage. Unfortunately, the changes in process configuration are accompanied by the adverse effect of capital cost. Therefore a trade-off of energy savings and additional investment expenditure arises. Using a shot-cut cost calculation, it is possible to make the best decision on the distillation process configuration for the recovery of iso-butane from an LPG stream.

1. Introduction

Distillation is one of the most popular processes in many recent industries. There is no doubt that distillation is also a highly energy-intensive process. It needs a lot of energy for operating a distillation column, however a large portion of demanded energy is not used properly leading to not only increasing the operating cost but also wasting the energy source, the shortage of which has been raising an alarming issue for recent decades. This is because energy almost comes from fossil fuel.

In this context, there have been a lot of optimizations and modifications in targeting of an energy efficient usage of distillation columns. However, this is definitely a very complex assignment. In order to improve the energy efficiency, the heat integration was first introduced almost 70 years ago (Amiya, 2010). So far, various heat integrated distillation schemes have been proposed. A great number of process configurations have been considered including combination of columns, changing the number of stages or the reflux ratio, feeding at different tray, using of pump around, side condenser and side reboiler, etc. There are many publications dealing with calculation and application of the so-called minimum thermodynamic condition column configuration (Filipe, 2011). Besides, Pinch Technology has been developed to be applicable to both new design and retrofit situations. Firstly Pinch Analysis for stand-alone modification of distillation column is considered, followed by principles for appropriate integration of

distillation columns with the remaining process. A tool that is used for column thermal analysis is called the Column Grand Composite Curve (CGCC). In order to obtain a CGCC, a converged column simulation is required, then necessary column data is extracted on a stage-wise basis. CGCC provides a thermal profile for a column and is used to identify appropriate targets for column modifications such as side condenser and side reboiler. CGCC relates to minimum thermodynamic loss in a column or an ideal column such which requires infinite number of stages and infinite number of side condensers and side reboilers.

In many situations it is possible to further improve the overall energy efficiency of the process by appropriate integration of the column with the background process. Appropriate column integration can provide substantial energy benefits. The combinations of different simple tasks to achieve hybrid tasks are considered as well. The concept of a task was first discussed and presented by Hendry and Hughes (1972), who focused on the investigation of the simple distillation columns. A simple task separation features a single feed with two products and a single light and heavy key component respectively. Hybrid tasks are used to accommodate complex configurations such as side-rectifiers, side-strippers, prefractionators, Petlyuk columns, dividing wall columns, vapour side-draw columns and liquid side-draw columns. Concepts for decomposing complex columns into an assembly of simple columns with thermodynamic equivalence are presented.

Figure 1 shows the combinations of two simple tasks in order to transform into a hybrid complex. There are two distillation columns on the left side which is so-called direct sequence configuration. The first column have a task of separating the lighter key components as an overhead product and the remaining portion as a bottom product which is fed into the second column to separate the intermediate and the heavier components. On the contrary, the right side of Figure 1 exposes an indirect sequence configuration where the heavier key components are firstly separated then the same manner for intermediate and lighter key components takes place in the second column.

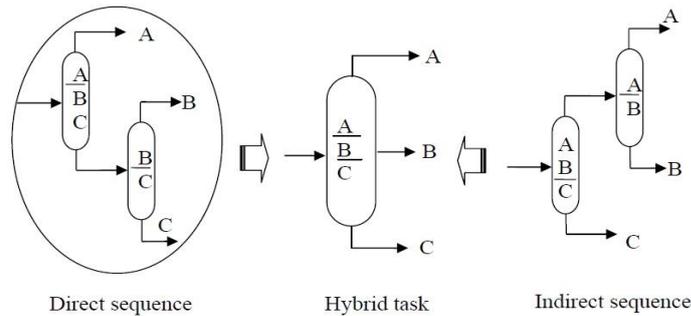


Figure 1: Combinations of two simple tasks into a hybrid task

The hybrid task of only one column revealed in the middle of Figure 1 is thermodynamically equivalent to both adjacent configurations. In this work, it is simplistically called as a conventional distillation configuration in order to distinguish from other configurations. That is a single side-draw column, particularly liquid side-draw column. The equivalent arrangement for a liquid side-draw column is shown in Figure 2. Liquid side-draw columns are obtained from the combination of two indirectly sequenced simple columns. The leading task in the indirect combination is the leading split of the liquid side-draw column. The available vapour then is used in the upper supplementary rectifying section to separate the light product (LP) from intermediate product (IP). However, they have fewer column sections and cannot achieve all purity and/or recovery levels without significant penalty on the reflux. This is proved in the simulation result for this conventional distillation configuration.

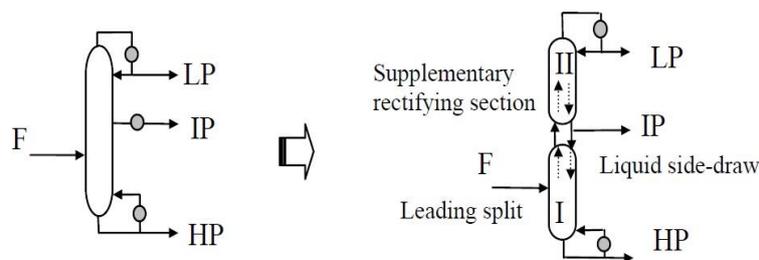


Figure 2: Thermodynamic equivalence of a liquid side-draw column

In the scope of combination simple columns into a hybrid task with side-draw product, one inventive configuration might be an excellent alternative choice to consider is that dividing wall column. The overall configuration of the Petlyuk column is quite similar to a product side-draw column with three product streams: one overhead stream, one bottom stream and another is a side-draw stream. Figures 3 and Figure 4 show the Petlyuk and the dividing wall column. Both of them have a thermodynamically equivalent configuration revealed by the assembly of three simple columns on the right side of Figure 3: one column with a partial condenser and a partial reboiler (I), two simple distillation columns with liquid side-draw (II) and vapour side-draw (III). As can be seen in Figure 4, the construction of the Petlyuk column may be carried out in a single shell with a dividing wall installed to separate the prefractionation from the main column section. Therefore, the so-called dividing wall column can save the capital investment by around 30 % (Dohare et. al., 2015).

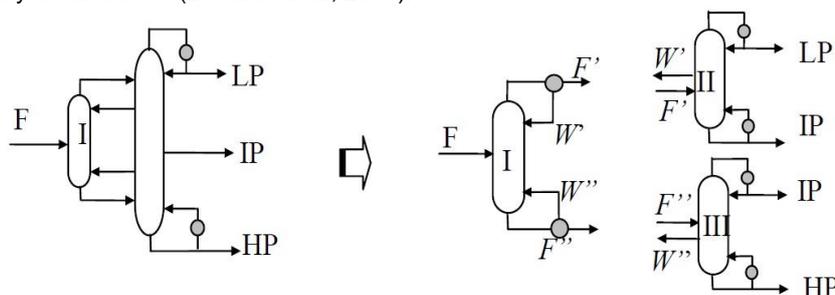


Figure 3: Thermodynamic equivalence of Petlyuk column

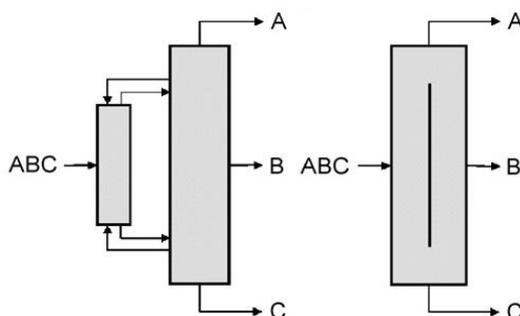


Figure 4: A middle-wall dividing wall column

The motivation of this work is analyse various configurations of distillation system, evaluating how much energy each configuration requires from the utility system. Moreover, it can assess not only how much energy need to be supplied, but also how energy is used by each of configurations. For many years, the first law of thermodynamics was believed as a suitable tool for evaluating the energy efficiency of processes. According to the First law, energy can neither be created nor be destroyed. That is always correct, however it is not sufficient to assert that the energy is used properly for a process. It is insisted that the quality of the energy always decreases as long as an energetic process continues. Therefore, it has become clearer that the quality of energy used in a process can be analysed by the second law of thermodynamics. Exergy analysis based on the second law of thermodynamics is a direct measurement of quality and efficient use of energy. Additionally, exergy is also an excellent tool for process optimization. The exergy of a system is defined as the amount of work obtainable when some matter is brought to a state thermodynamic equilibrium with the common components of the natural surroundings by means of reversible processes, involving interaction only with above mentioned components of nature Caballero, 2014) and later (Gourmelon, 2015). The use of CGCC to find the minimum exergy loss was successfully studied on a rectification column network (Markowski, 2014). Furthermore, exergy and pinch analysis could be combined as a method to reduce shaft work and to increase the exergy target (Thasai, 2015). With some assumptions, exergy value of a stream can be calculated by (Shin et. al., 2015):

$$Ex_{str} = H - T_0S \quad (1)$$

where H and S are the enthalpy and entropy of the stream at a particular state of the stream respectively and T_0 is the ambient temperature. Obviously, enthalpy and entropy both these properties are direct

functions of state, thus the exergy is also a property of a system and is a function of state as well. When the system moves from State 1 to State 2, the exergy change of the system is given by (Shin et. al., 2015)

$$\Delta Ex = Ex_2 - Ex_1 = (H_2 - T_0 S_2) - (H_1 - T_0 S_1) = (H_2 - H_1) - T_0 (S_2 - S_1) = \Delta H - T_0 \Delta S \quad (2)$$

Exergy transfer accompanying heat transfer is defined as (Shin et. al., 2015)

$$Ex_Q = \int_1^2 \left(1 - \frac{T_0}{T_b} \right) \delta Q \quad (3)$$

T_b denotes the temperature on the system boundary where δQ occurs. Both mentioned T_b and δQ appear within the entropy balance which originates from the second law of thermodynamics. It says that the change in the amount of entropy contained within a system during a time interval equals the net amount of entropy transferred in across the boundary of the system plus the amount of entropy produced within the system

$$\Delta S = S_2 - S_1 = \int_1^2 \left(\frac{\delta Q}{T} \right)_b + \sigma \quad (4)$$

Here the subscript b signals that the integral is calculated at the system boundary. The term σ accounts for entropy produced within the system by internal irreversibility. For a distillation column, the minimum amount of work required for the separation is equal to the difference between the exergy of the product streams and that of the feed stream (Shin et. al., 2015)

$$\Delta Ex_{str} = \sum_{product} Ex - \sum_{feed} Ex = Ex_{top} + Ex_{side} + Ex_{btm} - Ex_{feed} \quad (5)$$

A distillation column can be considered as a heat engine where heat from a high temperature source is transferred to a low temperature sink. Instead of mechanical work (shaft work), however, a separation work is generated by this model of heat engine. The work required for separation is supplied by the utility system, particularly for distillation column is that exergy input at the reboiler and exergy leaving in the condenser (Shin et. al., 2015)

$$\Delta Ex_{util} = Ex_{reb} - Ex_{cond} = Q_{reb} \left(1 - \frac{T_0}{T_{reb}} \right) - Q_{cond} \left(1 - \frac{T_0}{T_{cond}} \right) \quad (6)$$

The exergy loss of a column therefore can be calculated by performing a simple overall exergy balance across a volume control that is the column. By definition, the exergy loss is the difference between the summed exergy entering the column and the summed exergy leaving the column (Shin et. al., 2015)

$$\begin{aligned} Ex_{loss} &= \sum Ex_{in} - \sum Ex_{out} = \Delta Ex_{util} - \Delta Ex_{str} \\ &= Q_{reb} \left(1 - \frac{T_0}{T_{reb}} \right) - Q_{cond} \left(1 - \frac{T_0}{T_{cond}} \right) + Ex_{feed} - Ex_{top} - Ex_{side} - Ex_{btm} \end{aligned} \quad (7)$$

Obviously, in case of a reversible distillation column, there is an absence of irreversibility, the exergy loss thus is equal to zero. The minimum exergy requirement for the separation would be given by

$$\Delta Ex_{util, min} = \Delta Ex_{str} \quad (8)$$

There is no reversible column available in all real cases and the exergy required is far above the thermodynamic minimum.

2. Case studies

An LPG stream from Dinh Co gas processing plant in Ba Ria Vung Tau, Vietnam was used as a feed with the composition as following

Table 1: LPG composition

Component	Mole fraction (%)
ethane	1.81
propane	64.51
iso-butane	13.77
n-butane	18.62
neo-pentane	0.07
iso-pentane	1.04
n-pentane	0.18

The feed is at 16 bar, 60 °C with the flow rate of 21,800 kg/h. Three configurations were investigated and analysed. They are a conventional configuration (one side-draw column), a direct sequence configuration (two simple columns in series) and a dividing wall column. Propane is treated as the light key component, iso-butane is the intermedia (contributing) component and n-butane is the heavy key component.

2.1 Configuration I

The distillation column was simulated to operate at 9 bar. Thus the feed was expanded to 9 bar, temperature was about 37 °C and vapour fraction was 37.4 %. The interested iso-butane content in the liquid side-draw product was up to 95 mole %. Table 2 shows the operating parameters for all of configurations explored in this study.

Table 2: Operating parameters of configurations

Operating parameters	Configuration I	Configuration II		Configuration III	
		1 st column	2 nd column	Prefractionator	Main-column
Number of stage	97	35	63	28	87
Feed stage	90 th	16 th	39 th	3 rd	6 th and 69 th
Side-draw stage	25 th	--	--	--	27 th
Top pressure (bar)	7.96	15.80	6.55	8.96	8.76
Bottom pressure (bar)	9.30	16.30	7.45	9.35	9.60
Reflux ratio	20	1.83	9.892	4	5.274

2.2 Configuration II

In this configuration, two simple distillation columns were used in direct sequence. Most of the key component was available in the top stream of the first column and the bottom stream was the mixture of butane. This bottom stream was fed into the second column to separate iso-butane as the top product from n-butane contained mainly in the bottom product. The specification of iso-butane content was also up to 95 % mol.

2.3 Configuration III

This configuration considered using a dividing wall column which was thermodynamically equivalent to two columns mentioned in the above introduction section. The iso-butane in this model was recovered mostly in the side-draw product stream with 95 % mole iso-butane content. A DWC is simulated based on the configuration on the right side in Figure 3, a prefractionator as column I and there is one distillation column, instead of two columns II and III, as a main column. The duty of the reboiler and condenser of DWC are the sum of two reboilers and two condensers of two columns in simulation, respectively.

3. Results and discussion

The parameters that is necessary for calculating such as enthalpy, entropy, composition, flow rate, heat rate, etc. were exported from the data result of Aspen HYSYS®. The results of exergy analysis for each of configuration mentioned in Table 3. As can be seen, the exergy loss value of configuration II is the least among three configurations suggested to investigate. It says that the direct sequence of two simple distillation columns which could recover iso-butane from LPG with the same iso-butane content of about 95 % mole in the product stream use supplied energy most efficiently. In comparison among three investigated configurations, one can see that using one conventional column with a side-draw product requires a much greater amount of energy. However, the minimum energy that is necessary for separation is much less than total energy supplied for this configuration. This conclusion is stated due to the calculated exergy loss value shown in Table 3.

The same goal of all these three configurations is that recovering iso-butane from LPG, it is therefore believed that there is no major difference over the amount of work for separation of iso-butane.

Table 3: Results of configurations

Result	Configuration I	Configuration II		Configuration III
		1 st column	2 nd column	
Condenser duty (kJ/h)	99,418,737.6	11,034,824.2	11,836,098.5	51,426,864.9
Duty of reboiler (kJ/h)	96,866,603.2	10,336,002.7	10,839,490.7	49,012,617.6
Exergy loss (kJ/h)	17,041,791.1	3,464,638.3		6,899,865.4

In real cases the work consumed by the utility system has to be always greater than the minimum work required by separation. As above mentioned, this difference between the amount of work consumed by utilities and that of separation required is exergy loss. Looking at the exergy loss values of configuration II and III, they are about 3.5 GJ/h and 6.9 GJ/h. It means, due to quite a similar amount of required separating work, it needs more 3.5 GJ/h in order to operate the configuration II or 6.9 GJ/h more to run the system of configuration III. However, configuration I demands much more energy to be able to recover iso-butane. A large portion of supplied energy is wastefully used which is indicated by a much higher exergy loss, around 17 GJ/h compared to 3.5 or 6.9 GJ/h. Nevertheless, one of advantages from configuration I can be imagined is that it might spend a lower expenditure to build this system because there is only one column. Obviously there is a trade-off of energy saving concept and the capital cost. A short-cut cost calculation is carried out based on assumptions of material price, build-up price, electricity price.

Table 4: Short-cut cost calculation result

Cost	Configuration I	Configuration II		Configuration III
		1 st column	2 nd column	
Capital cost (USD)	485,000	175,000	315,000	575,000
		490,000		
Operating cost (USD/y)	438,370,594	47,728,180	50,642,149	224,314,843
		98,370,329		

A brief calculation of cost with some simplified assumptions shows that the operating cost is much higher than the build-up cost of columns. This is because there is a considerably great amount of energy consumed to meet the requirement of purity of iso-butane in the separated product. One could reference both the economic aspect and energy saving concept to make a suitable decision for the choice of configuration II.

4. Conclusion

This study shows up three different ways to recover iso-butane from an LPG with the purity of iso-butane in the separated product up to 95 mole %. The iso-butane recovery ratio is recorded about 94.68 % out of the iso-butane content in the feed source. An arrangement of two distillation columns in direct sequence is indicated as the best choice compared to two others investigated based on exergy analysis and a brief cost calculation. For the same criterion on products, technology could solve it well by many means. Nevertheless, the efficiency is much more important represented by the loss of energy quality, namely exergy. Configuration II suggests a proper way of energy utilization for the purpose of iso-butane recovery.

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