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Selection of Economically Optimum Operating Conditions in Complex Distillation Systems for NGL Fractionation Processes

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ABSTRACT

Implementation of innovative distillation systems in multicomponent distillation design is a complex task because of multitude design variables. Operating pressure is one of the most prominent and effective variables in the distillation columns, which affects capital and operating costs directly. Many heuristic and optimization based methods are presented to find optimal operating conditions of distillation columns. Since the natural gas liquids, NGL, fractionation process is a costly and an energy demand intensive process, the design and operation of these units may affect many important petrochemicals supply chain and whole natural gas processing plant. Herein a comparison has been made between an easy to use heuristic design method and a stochastic based optimization method with genetic algorithm to design the simple and complex multicomponent distillation columns sequences for NGL fractionation processes. The results demonstrate the heuristic method is faster but in complex distillation systems, is inaccurate. In the studied case of the NGL fractionation process, the calculated column pressure by a heuristic method showed up to 40% different in comparisons against stochastic optimization results. This error leads to a 3% increase of the total annual costs in the heuristic method, which may have a significant impact on the final design and change the evaluation distillation scenarios because of cumulative error effects.

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1. Introduction

Separation processes are necessary in many (petro-) chemical processes and account for an estimated up to 70% of plant operations and capital costs (Nezhadfard et al. 2018). Over the recent decades, because of the increasing energy costs and importance of greenhouse gas emissions reductions, improving the gas processing and petrochemical processes have been widely studied (Ivakpour, Kasiri, 2009; Kiss, 2014).Increasing the process efficiency by using sustainable designs for conventional processes is a prominent solution for the global warming problem (Shahandeh et al. 2015). One of the energy demanding processes is the natural gas liquids (NGL) fractionation process. The natural gas obtained from field processing units after dehydration and treating, passes the NGL extraction unit and NGL enters the fractionation unit as under pressure feed stream (Manley 1998). The objective of this unit is fractionating the hydrocarbons with a train of distillation columns. The main products of this process are ethane, propane, butanes, and condensate which are separated by three distillation columns in a direct arrangement as the conventional design (Yoo et al. 2016). Innovative designs for this process are studied for using complex distillation columns, replacement by divided wall columns and effect of the operating variables in the design stage (Halvorsen et al. 2016; Long et al. 2013).

The high number of variables in the design of distillation columns such as pressure, reflux ratio, number of stages, feed and side streams stage locations and stream flow rates bearing about a complex design problem. In addition, the economic design and optimization of distillation systems are complicated because of dealing with non-convex cost functions and the trade-off between capital and operating costs (Lee at al. 2018). Pressure has a major influence on capital cost in terms of allowable stress of materials and wall thickness also on operating costs because of phase equilibrium and column temperatures, which affect utility costs and process configurations. Since the low-temperature distillation is preferred, columns pressures are determined by a desire to use the cold utility in the condenser as a heuristic rule (Luyben et al. 2016). Following this rule leads to the use of the inexpensive cold utility at the lowest possible pressure. On the other hand, the increase of the column pressure increases the bottom temperature and that may lead to high-pressure steam demand in reboilers. Higher column pressure equivalent to higher capital costs, interactions not considered in heuristic pressure determination methods. Accordingly, the optimization-based methods are developed to solve the current issue use stochastic optimization to minimize a desired objective function like total annual costs (Tahouni et al. 2010).

Many parameters might affect the NGL fractionation process operation in addition to column pressure. For example, the reflux ratio is one of the important distillation parameters that affect condenser and reboiler heat duty and column diameter as well as column height. The feed stage might change the temperature profile in the column and the side steam stage might affect product composition.

Finding the optimal operation conditions is very important in multicomponent distillation systems, especially in complex distillation configurations because of the reciprocal influence of operating variable, which brings about a complex problem. In the NGL fractionation processes, the desired pure products are separated in a multicomponent distillation system. The simple and complex competitive distillation sequences are presented for four-component distillations in which the simple sequences are used as simple distillation columns with one reboiler and condenser, one feed and two products and complex sequences are used as complex columns with more than one feed and side stream products (Khalili-Garakani et al. 2016 a).

Herein a comparison was made between the heuristic method and genetic algorithm (GA) optimization for simple and complex four-component distillation systems in order to investigate the effects of operating pressure on the total annual costs in the NGL fractionation process. Also, the impact of the accuracy of the optimization method on complex distillation systems design parameters and operation and capital costs are scrutinized.

2. Methods

As mentioned, the pressure is the most influential variable on the operating condition of the distillation systems and should be determined in the first design stage. The utilized heuristic method for operating pressure selection starts the analysis algorithm for the first column of the sequence and increases the operating pressure from atmospheric pressure to maximum allowable pressure (2861 kPa in this case) and calculate the condenser temperature to find the inexpensive cooling water or refrigerant based on the table 1a values. The procedure is repeated for other distillation columns of the sequence and the operating pressures are determined. The heuristic approach studies the operation conditions of the columns individually and does not consider the reciprocally influencing effects of columns on the sequence.

Table 1. Utility Specifications and Costs (Seider et al. 2017)

a) Cooling Utilities

Utilities	Temperature (°C)	Price ($/GJ)
Cooling water	25	0.675
Refrigerant1	-12	6.470
Refrigerant2	-35	13.17
Refrigerant3	-68	23.30

b) Heating Utilities

Utilities	Pressure (kPa)	Temperature (°C)	Price ($/ton)
Low pressure steam	350	148	13.20
Medium pressure steam	1050	185	15.30
High pressure steam	3100	238	17.60

The optimization-based approach, analyzes all columns of the sequence simultaneously by the genetic algorithm. The optimization variables are the operating pressures of the columns and the objective function of minimization is the total annual cost (TAC) of the sequence. The TAC ($/year) is calculated by Eq. 1 where C_{Cap} is the capital cost, C_{Op} is the operating cost, i is the interest rate (0.1) and n is the plant lifetime (10 years). The capital cost of a column is calculated by the summation of condenser cost (Eq. 2), reboiler cost (Eq. 3), vessel cost (Eq. 4) and tray costs for sieve trays (Eq. 5) where A (m^2) is the heat exchange area, W (kg) is the vessel weight, D_i (m) is the column diameter and N_T is the number of trays [13]. The column diameters for shortcut distillation columns are calculated by Eq. 6 where V is the vapor flow rate, RR is the reflux ratio, T_D is the distillate temperature and P is the column pressure (Cui et al. 2018).

The optimizer varies the shortcut columns operating pressures to calculate the reflux ratio, number of trays, feed and product locations, as well as reboiler and condenser heat duties by the Aspen plus. The results of the simulation are returned to the optimizer and TAC is calculated. GA operators generate the new individuals based on the results of these reciprocal calculations. But in Heuristic method the operating pressure of each column is increased laniary and step by step and all above mentioned parameters are calculate for each pressure based on the simulation results. These automatic data transformations and calculations between MATLAB and Aspen Plus are done with Aspen and MATLAB linking methods (Appendix A).

$$TAC = C_{Cap} \times \frac{i(i+1)^n}{(i+1)^n - 1} + C_{Op} \tag{1}$$

$$C_{cond} = \exp\{11.4185 - 0.9228[\ln(10.76A)] + 0.09861[\ln(10.76A)]^2\} \tag{2}$$

$$C_{reb} = \exp\{12.3310 - 0.8709[\ln(10.76A)] + 0.09005[\ln(10.76A)]^2\} \tag{3}$$

$$C_V = \exp\{10.5449 - 0.4672[\ln(W)] + 0.05482[\ln(W)]^2\} \tag{4}$$

$$C_T = 468\exp(0.486 \times D_i) \times N_T \tag{5}$$

$$D_C = \left[\left(\frac{4}{\pi V}\right) \times (D) \times (RR+1) \times (22.4) \times \left(\frac{T_D}{273}\right) \times \left(\frac{1}{P}\right) \times \left(\frac{1}{3600}\right)\right]^{0.5} \tag{6}$$

Hyper-parameters of the GA such as population size and crossover fraction are optimized based on the order of issue and the optimization problem is solved multiple times to assure the results are globally optimum. The Winn-Underwood-Gilliland equations within the Aspen plus shortcut simulator are used to carry out the simulation of distillation sequence using Peng-Robinson equation of state. The simulation of the complex configurations is carried out by decomposing the complex distillation columns into simple thermodynamically equivalent units (Wang, Smith, 2005). The GA toolbox of the Matlab manipulates the simulator through Aspen-Matlab linking methods. The GA generates a population of operating pressures for all distillation columns and sends to Aspen plus simulator. The Aspen plus solves the simulation for fixed feed and products specifications and calculates the heat duties, temperature profiles, number of trays and reflux ratio for all columns. The simulation results are transferred to the Matlab where the GA calculates the TAC. These calculations continue until the GA is converged to the optimum TAC of a sequence.

The distillation column sequences for four-component systems with three distillation columns are illustrated in Fig. 1. In these sequences, the feed stream is demonstrated by {F} and distillate, bottom, and side stream products are demonstrated by {I}, {II}, {S} respectively. The possible simple and complex distillation scenarios are generated by the separation matrix algorithm (Khalili-Garakani et al. 2016 b).

3. Casestudy

A significant portion of natural gas is NGL, which has a high economic value. The NGL fractionation process separates the ethane, propane, butanes, and condensate with the desired specification from natural gas liquids feedstock with three distillation columns. The feed and the products specifications of this process are shown in table 2. The feed stream pressure and temperature are 4238 (kPa) and 29.4 (ºC) respectively. The main products are specified by A as ethane-rich product with 0.99% recovery of methane and ethane, B with 0.98% propane purity, C with 0.98% isobutene and normal butane purity and D as condensate with 0.99% pentanes recovery. The feed and products specifications are kept the same in all distillation scenarios.

Table 2. Feed and Product Specifications of NGL Fractionation Process (Yoo et al. 2016)

Components	Feed (kmol/hr)	A (molfrac)	B (molfrac)	C (molfrac)	D (molfrac)
Methane	61.9	0.02			
Ethane	2901.1	0.97	0.01		
Propane	1980.3	0.01	0.98	0.01	
i-Butane	461.4		0.01	0.31	
n-Butane	984.4			0.67	0.01
i-Pentane	286.4			0.01	0.36
n-Pentane	202.5				0.26
n-Hexane	203.9				0.26
n-Heptane	90.9				0.11

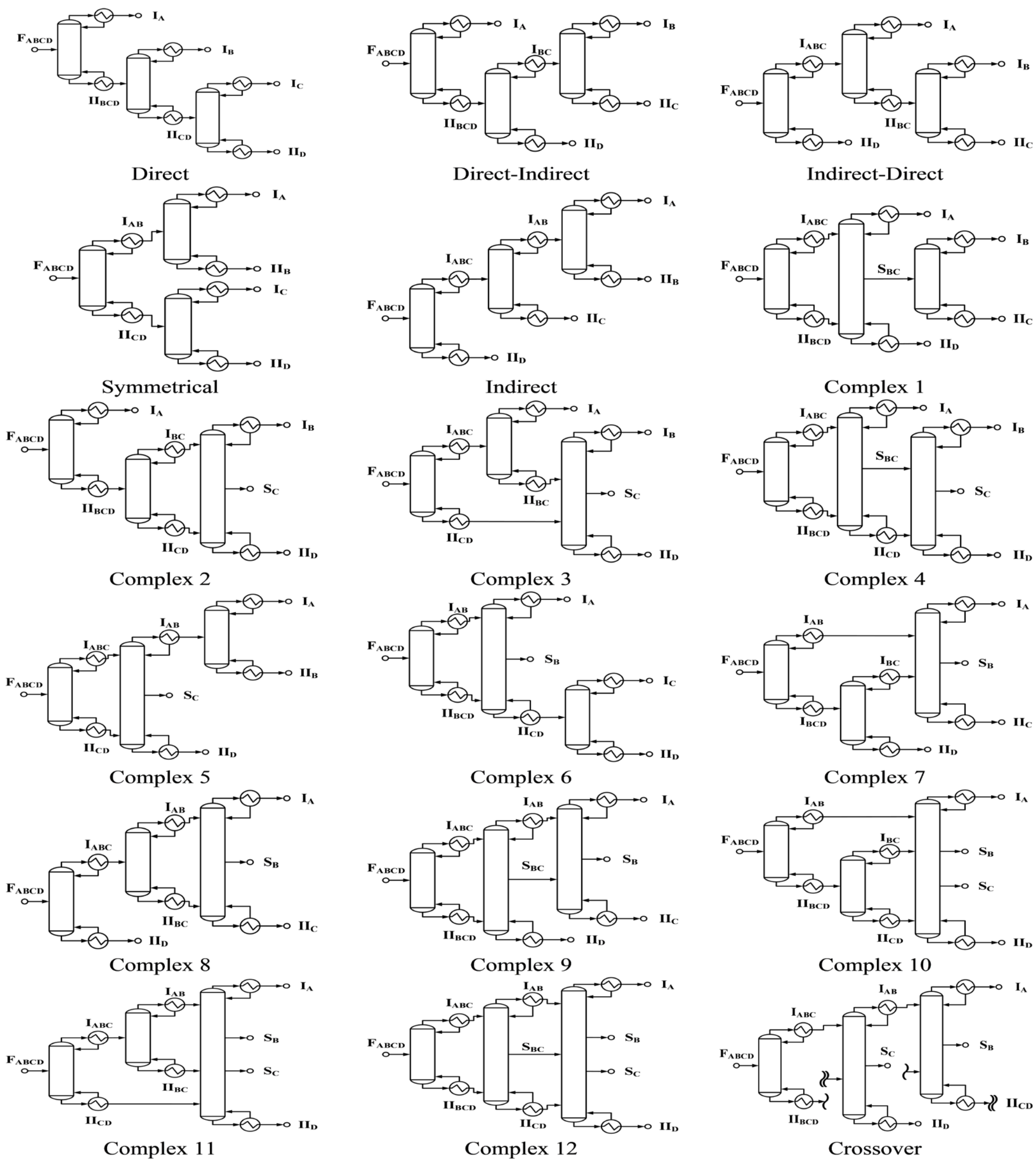

Figure 1. Distillation Columns Configurations for Four-Component Systems

4. Results and Discussions

The columns operating pressures are calculated by heuristic and stochastic methods for all simple and complex distillation scenarios. The TAC function is calculated for each sequence in the optimum pressure of two methods and the results shown in Fig. 2. In the heuristic method, the pressure of each column changed from atmospheric pressure (101 kPa) with a step size of one kPa to find the suitable condenser utility type. The sequence pressure is calculated simultaneously for all columns to minimize the TAC of the sequence in the GA method. The population size of the GA is 50 individuals in each generation and crossover fraction is 0.8. The results of the two methods for simple sequences including direct, direct-indirect, indirect-direct, symmetrical and indirect are reasonably similar. In the complex sequences, some of the calculated pressures by the two methods are different. These lead to different TACs. In all cases, the TAC of the GA is less than or equal to the heuristic method result. The largest differences are observed in Complex4, Complex9, Complex11, Complex12 and Crossover sequences. The computational time for each sequence in the heuristic method has been one-sixth of the genetic algorithm.

The difference between this two algorithm results might affect sequences rankings and the shortcut simulation cannot indicate the best sequence globally but the rigorous simulation and optimization results of this process demonstrates the Complex2 sequence is de best distillation configuration for NGL fractionation process (Tamuzi et al. 2020).

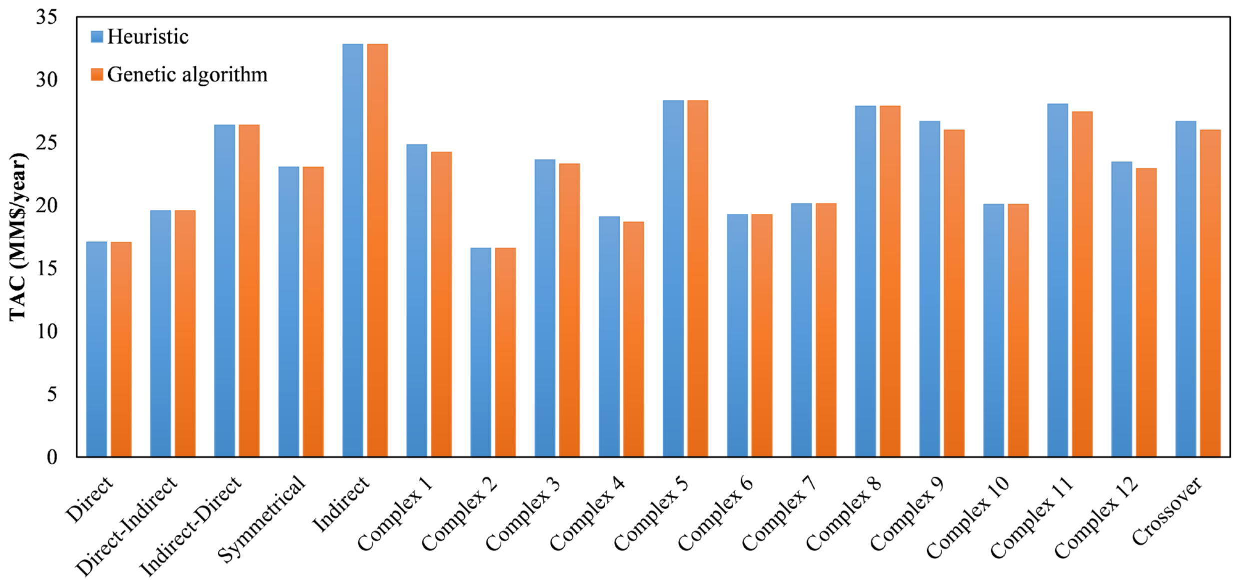

Figure 2. The Calculated TAC from Heuristic and Genetic Algorithm Methods for Distillation Sequences

The Complex9 sequence is illustrated in Fig. 3a. The calculated TAC for this sequence by the heuristic method is 3% greater than GA results. Fig. 3b shows the columns operating pressure of this sequence. The second and third columns pressures are the same in two methods. For the first column, the heuristic algorithm has been stopped in 1650 kPa but the GA has chosen 2860 kPa as optimum pressure. A closer look at the effect of the first column's operating pressure on the column and the configuration performance has been made.

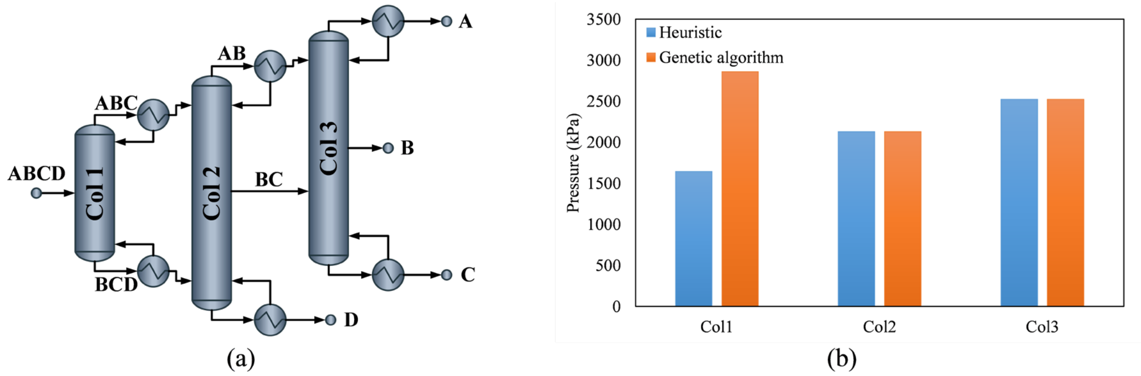

Figure 3. The Sequence with Highest Error (a) and Calculated Column Pressures by Two Methods (b)

The first column (Col1) of the sequence shown in Fig. 3a is used as a pre-flash column to separate all of A component with a part of B, C components as non-sharp distillate stream and all of the condensates (D) with a part of B, C as non-sharp bottom product. The Col1's products are the feed streams of other columns of the sequence. The impact of this column operating pressure on the condenser and reboiler temperature is shown in Fig. 4. The dotted lines illustrate the temperature of each utility which can be used as heating or cooling proposes in the reboiler and condenser. The low-pressure steam can be used in reboiler for all of the pressure range, but the condenser utility is interdependent to the column pressure. Increasing the column pressure increases the condenser and reboiler temperature and makes possible using the inexpensive utility in the condenser. Because of the non-sharp separation in the Col1, the reboiler temperature is always lower than low-pressure steam but for the separation of heavier hydrocarbons, the trade-off of reboiler and condenser temperature is more important in economic optimization.

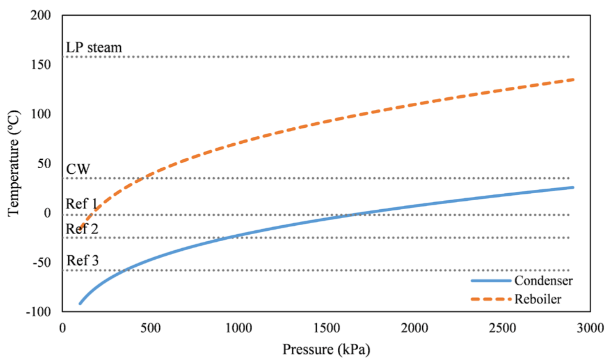

Figure 4. The Impact of Col1's Pressure on Condenser and Reboiler Temperatures

The shortcut design of distillation column utilizes the thermodynamic equations to estimate column operating and geometry. Accordingly, the column pressure affects components relative volatilities and the number of theoretical stages, minimum reflux ratio and so on. The effect of the column pressure on reflux ratio for Col1 is shown in Fig. 5a. Increasing the column pressure from atmospheric pressure to 420 kPa decreases the reflux ratio and then increases until 2860 kPa. Increasing the reflux ratio changes the column internal flow rates and the vapor flow rate directly affects the column diameter but as seen in Eq. 6 the column diameter inversely changed with pressure. The impact of the pressure on the column diameter is shown in Fig. 5b. This trade-off, cause the minimum column diameter at 2520 kPa. Another important parameter in the distillation column design is the number of stages. As shown in Fig. 5c, the number of actual stages of the same separation, increases with column pressure. Considering all of these parameters, the column capital cost increases with operating pressure.

The NGL fractionation unit is an energy demanding distillation process and a major part of the TAC belongs to the unit operating costs. Fig. 5d shows the impact of column operating pressure on the annual operating cost. From atmospheric pressure to 1650 kPa, the capital cost decreased with the increase of the pressure, but then the capital cost mildly increased. According to the results and considering the first column, the best operating pressure of this column is 1650 kPa. The heuristic method shows the same result for this column as the best operating pressure. In 1650 kPa, using the inexpensive utilities is possible, the operating cost of Col1 is minimized and the capital cost is as low as possible at pressures greater than 1650 kPa. However, as the main objective of this research, the operating conditions of a column may affect the entire unit and this should be investigated.

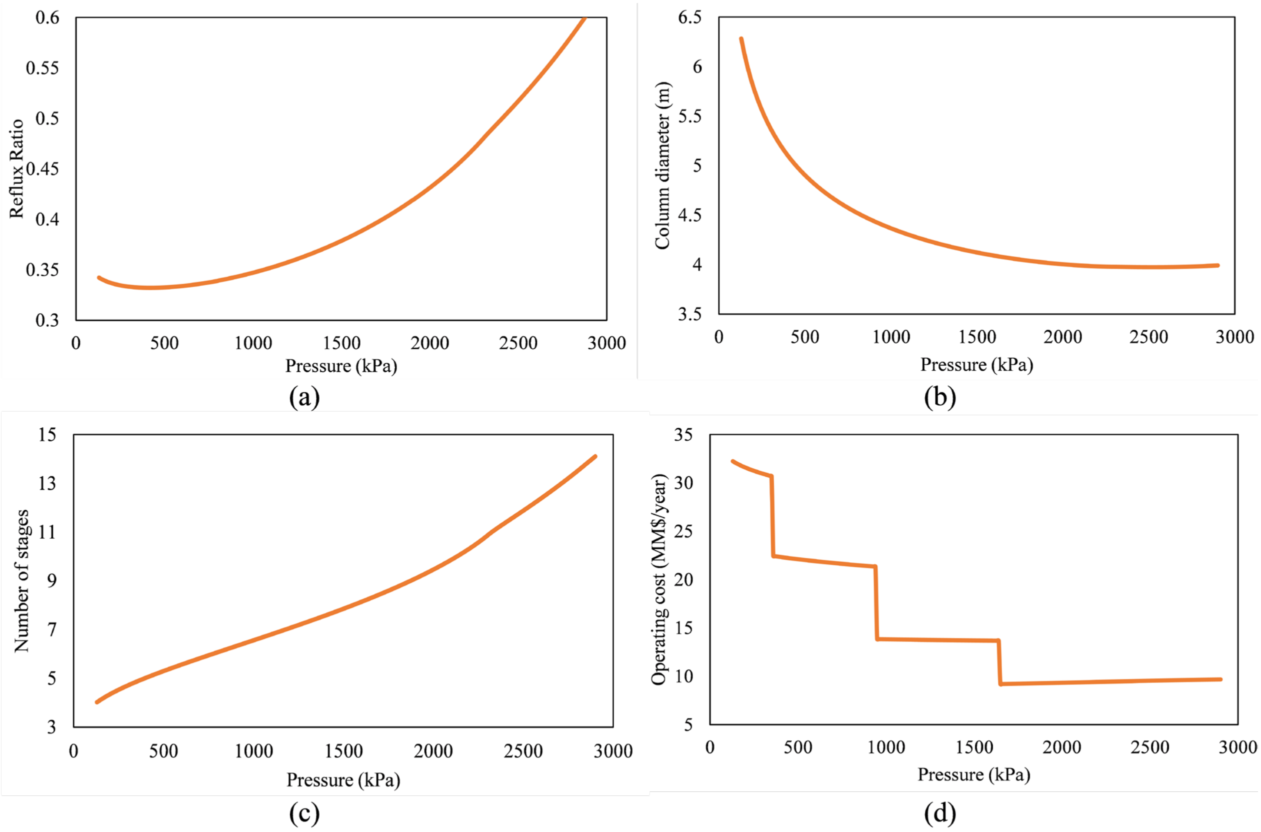

Figure 5. The Impact of the Col1's Pressure on the Reflux ratio (a), the Column Diameter (b), the Number of Stages (c) and the Column Operating Cost (d)

As it mentioned the columns of a distillation sequence are not independent, and the columns interplay effects are more in complex configurations. TAC as a comprehensive objective function can be useful in investigating the effect of operating conditions on the distillation unit economy. Fig. 6 shows the impact of the operating pressure of Col1 from Fig. 3 on the TAC of that column and whole sequence. Increasing the pressure decreases the TAC of the Col1 and the sequence until 1650 kPa. After that, the Col1's TAC starts to increase from 9.38 MM$/year at 1650 kPa to 9.92 MM$/year at 2860 kPa but the sequence shows different behavior and the TAC increased 0.5 MM$/year with increasing the pressure. This happens because increasing the column pressure increases the column products temperature those are the feed streams of the next columns. Increasing the temperature of the middle streams can reduce the cost of other columns and compensate for the increase in the cost of the first column.

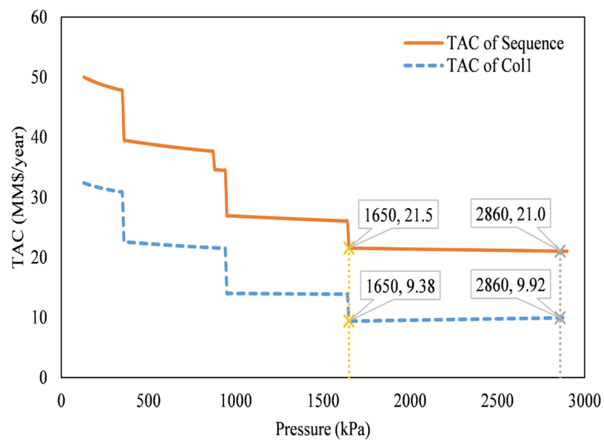

Figure 6. The Impact of the Pressure on the TAC of the First Column and the Sequence

5. Conclusions

The energy consumption and environmental pollutions subjects are so important in petrochemical upstream units like NGL fractionation plants. Using innovative designs instead of conventional processes may be useful and improve the operation of the unit. The design of these processes is more complex and need to use computer-aided simulation, optimization and design methods. For this purpose, this research investigates the impact of columns operating pressure on the plant operation and economy. The two methods of heuristic rules and stochastic optimization for the design of simple and complex distillation configurations of the NGL fractionation process are compared.

Simulation of distillation sequences is carried out by aspen plus shortcut columns and the Matlab used as the optimizer for manipulating the simulator by Aspen-Matlab linking method. The results illustrate the heuristic method can be used as a quick calculation in simple configurations, but in complex distillation sequences have some errors against stochastic optimization results. In the studied case of the NGL fractionation process, the calculated column pressure by a heuristic method showed up to 40% different in comparisons against stochastic optimization results. This error leads to a 3% increase of the total annual costs in the heuristic method, which may have a significant impact on the final design and change the evaluation distillation scenarios because of cumulative error effects.

Appendix A

Aspen and MATLAB linking methods (Example code)

```
Aspen=actxserver('Apwn.Document.36.0');
Aspen.invoke('InitFromArchive2','C:\Users\***.apw');
Aspen.visible=1
Aspen.SuppressDialogs=1;
Run2(aspen.Engine);
for P=P0:P
Aspen.Application.Tree.FindNode('\Data\Blocks\B1\Input\PRES').value=P;
Run2(Aspen.Engine);
X(i)=aspen.Application.Tree.FindNode('\Data\Streams\2\Output).value
Calculate TAC
end
```

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چکیـــــده

استفاده از طرح‌های نوآورانه در طراحی فرآیندهای تقطیر چند جزئی به دلیل تعداد بالای متغیرهای طراحی کاری بسیار پیچیده است. فشار یکی از پارامترهای عملیاتی مهم در برج‌های تقطیر است و به‌طور مستقیم بر هزینه‌های عملیاتی و سرمایه‌ای تأثیر گزار است. تاکنون روش‌های بسیاری شامل روش‌های ابتکاری و بهینه‌سازی برای یافتن فشار عملیاتی بهینه برج‌های تقطیر ارائه‌شده است. ازآنجاکه فرآیند تفکیک مایعات گاز طبیعی (NGL) یک فرآیند پرهزینه و پرمصرف ازنظر انرژی محسوب می‌شود، طراحی و بهره‌برداری از این واحد فرآیندی تأثیر قابل‌توجهی در زنجیره تأمین محصولات پتروشیمی و کل مجموعه فرآوری گاز طبیعی می‌گذارد. در این مقاله مقایسه‌ای بین روش طراحی ابتکاری برج‌های تقطیر و روش بهینه‌سازی تصادفی به کمک الگوریتم ژنتیک برای طراحی چیدمان‌های ساده و پیچیده برج‌های تقطیر در فرآیند تقطیر چند جزئی به‌منظور طراحی فرآیند تفکیک مایعات گاز طبیعی صورت گرفته است. نتایج این پژوهش نشان می‌دهد که روش ابتکاری عملکرد سریع‌تری نسبت به روش بهینه‌سازی دارد اما در چیدمان‌های پیچیده برج‌های تقطیر با مقداری خطا همراه است. در مطالعه موردی صورت گرفته برای فرآیند تفکیک NGL نتایج حاصل از بهینه‌سازی توسط روش ابتکاری اختلاف ۴۰درصدی در فشار محاسبه‌شده برای برخی از برج‌ها نسبت به روش بهینه‌سازی با الگوریتم ژنتیک نشان می‌دهد. این خطا باعث افزایش ۳ درصدی هزینه‌های سالانه چیدمان می‌شود که به دلیل خاصیت تجمعی خطا می‌تواند تأثیر قابل‌توجهی بر طراحی نهایی واحد گذاشته و حتی رتبه‌بندی نهایی چیدمان چیدمان‌ها را تغییر دهد.

واژگان کلیدی: تفکیک NGL، فشار عملیاتی، تقطیر چند جزئی، بهینه‌سازی فرآیند، قوانین ابتکاری