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Exergy Analysis and Heat Integration of Distillation Columns using Thermal Coupling Method for Separation of Ternary Mixture

Taraneh Mostofian*, Maryam Noori Keshtkar, Shohreh Ebrahimi

Department of Chemical and Petroleum Engineering, Sharif University of Technology, Azadi Street, Tehran, Iran

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ABSTRACT

Despite distillation's popularity in the industry, it is highly energy-intensive. Heat integration is therefore essential considering the recent energy crisis. This paper presents thermal coupling as an approach for separating the ternary mixture of n-pentane, n-hexane, and n-heptane. In this method, the first column supplies vapor to the second column while its reboiler is removed. The thermal coupling method is evaluated using two classical arrangements, direct and indirect with and without heat integration. Simulation of separation processes is carried out using Aspen HYSYS, and distillation columns are simulated using the rigorous solving method rather than the shortcut method. The simulation results are compared to those obtained using the shortcut method (minimum produced steam). Furthermore, exergy analysis is used for assessing processes in addition to energy analysis. It has been demonstrated that direct sequence provides better results than indirect sequence. Moreover, direct-thermal coupling is considered the most efficient process among the four investigated processes. It has been concluded that compared to the indirect process without heat integration, the direct-thermal coupling sequence can reduce energy consumption and exergy loss by 69% and 55%, respectively, as well as improve exergy efficiency by 9%.

1. Introduction

It is crucial to separate ternary mixture of n-pentane, n-hexane, and n-heptane. N-pentane is used in the laboratory and as a foaming agent in the production of polystyrene. N-hexane is also utilized in the dye and leather industries. Moreover, n-heptane is used to produce anesthetics. The first option for separating a ternary mixture of n-pentane, n-hexane, and n-heptane is distillation, which is by far the most commonly used method of separation in the industry. In order to separate ternary mixtures into pure components, two distillation columns are required, but these

Corresponding author. Tel.: +98 000; fax: +98 000.
E-mail address: taraneh.mostofian@gmail.com (T. Mostofian)

columns are energy-intensive. The recent energy crisis and environmental concerns make it imperative to optimize distillation columns' energy consumption [1–5].

Over the past decades, many studies have been conducted on the separation of ternary mixtures using distillation and also on optimizing their energy consumption adopting different methods including dividing wall column (DWC), vapor recompression (VRC), heat pump, heat-integrated distillation column (HIDiC), feed splitting and Multi-effect [6-10].

Babaie and Nasr Esfahany [9] evaluated the impact of feed splitting on three classical arrangements with and without heat integration in an effort to reduce the total annual cost (TAC). Separation of a ternary mixture including (propane, butane and pentane) using distillation column was selected as a case study. Parameters affecting TAC were calculated and optimized using genetic algorithm. It was observed that feed splitting with heat integration reduced the TAC considerably.

Cui et al. [11] investigated ten different separation processes including direct, indirect, and prefractionators with heat integration for separating a ternary mixture of Benzene, Toluene, and Xylene. It was observed that Combining two classical arrangements, indirect and prefractionator, resulted in the lowest total annual cost (TAC) due to a significant reduction in reboiler duty.

Wei et al. [12] studied three different separation processes including dividing wall column (DWC), fully thermal coupled (FTC), and conventional for separating a ternary mixture of, 3-dimethyloxetane, 3-chloro-2, 2-dimethylpropanol, methylcyclohexane. The conventional process consisted of two distillation columns arranged indirectly. The three processes were evaluated in terms of their environmental impact, thermodynamic efficiency, and economic feasibility. The results indicated that DWC had the highest economic appeal, while FTC had the highest thermodynamic efficacy and lowest CO_2 emissions.

Cui et al. [13] investigated the separation of a ternary mixture of methyl cyclopentane, cyclohexane, and lighter components using two methods, prefractionator and DWC. Results showed that the prefractionator process performed better in terms of cost efficiency while the DWC process had higher thermodynamic efficiency.

Javed et al. [14] studied the efficacy of the four different separation methods, conventional distillation column (CDC), internally heat-integrated distillation column (IHIDiC), externally heat-integrated double distillation column (EHIDIC), and vapor recompression (VRC) for separating ternary mixtures containing propane, iso-butane, and n-butane. Exergy analysis were conducted for all separation methods. It was determined that the VRC method had the highest exergy efficiency with 10.60%, whereas the IHIDiC method had the lowest exergy efficiency.

The purpose of this paper is to conduct a heat integration on the separation process of n-pentane, n-hexane, and n-heptane. Thermal coupling is employed as an approach to heat integration. Using this approach, the second distillation column's reboiler is removed and its vapor needs are met by the first column. In this study, two classical arrangements, direct and indirect with and without heat integration are simulated with Aspen HYSYS. Simulation results are then compared with those obtained by utilizing the shortcut V_{min} method. For all processes, this method compares the total amount of steam generated in the two distillation columns. Considering that energy consumption, environmental issues, and exergy losses are inextricably linked, exergy analysis is coupled with energy analysis for process assessment.

2. Case Study

This paper studies the separation of the ternary mixture of n-pentane, n-hexane, and n-heptane using distillation. Feed conditions are shown in Table 1 [1].

Table 1. Feed conditions

Parameter	Value
Pressure	470 kPa
Molar flow	100 kmol/h
Components mole fraction(n-pentane, n-hexane, n-heptane)	0.4, 0.2, 0.4
Vapor phase fraction	0

3. Distillation columns arrangement

There are two classical arrangements for separating the ternary mixture into pure components namely, direct and indirect. In the direct sequence, the light component exits from the first column, and the two other components are separated in the second column. While in the indirect sequence, the heavy component leaves the first column and the remaining components are separated in the second column [15].

4. Methods

Simulations of separating processes are carried out using Aspen HYSYS V.11. Modified HYSIM inside-out is used for calculating distillation columns. Moreover, the Peng-Robinson equation is employed for calculating component fugacity coefficients in liquid and vapor phases. Classical processes including direct and indirect are simulated with and without heat integration. In both cases, there are two distillation columns. In the direct arrangement, n-pentane is separated from the first column. The second column separates n-hexane and n-heptane. In the indirect arrangement, n-heptane leaves the first column as the top product while the two other components are separated in the second column. Thermal coupling method is employed for heat integrating of both direct and indirect arrangements. Using this method, steam from the first column is used to provide steam for the second column. This method allows the second column reboiler to be removed. In addition, a stream from the second column is recycled back into the first column, with the bottom product of this column leaves as a side stream.

4.1. Thermal coupling sequence

The thermal coupling method is recognized as one of the methods for heat integration utilized for the integration of heat in distillation columns, including direct, indirect, and prefractionator arrangements. Using this method, the condenser or reboiler of one column is removed, and the required steam is provided by the other column. In this study, the reboiler in the second column is removed, resulting in the second column being supplied with steam via the first column's output stream [16].

4.2. Exergy analysis

Exergy is defined as the maximum amount of work produced from a given amount of energy. The objective of this analysis is to calculate the exergy loss and efficiency associated with the processes. Exergy analysis is based on the second law of thermodynamics; therefore, it must be combined with energy analysis for a comprehensive evaluation of processes. Calculation of exergy losses is carried out using an energy balance for the system. The following equation illustrates how exergy loss is calculated [17–19].

$$I = \sum EX_{in} - \sum EX_{out} + EX_1 - EX_2 \quad (1)$$

where I is exergy loss and the indexes of in, out, 1, and 2 represent input, output, initial, and final streams of the system, respectively. At steady state, Eq. (1) is converted into Eq. (2):

$$I = \sum EX_{in} - \sum EX_{out} \quad (2)$$

Exergy input and output can include stream exergy, heat exergy, and work exergy, which are determined by Eq. (3) to (5).

$$EX_{stream} = (H - H_0) - T(S - S_0) \quad (3)$$

$$EX_Q = Q(1 - \frac{T_0}{T}) \quad (4)$$

$$EX_W = W \quad (5)$$

In the following equations, H is enthalpy, Q is heat, and W is work. T_0 is also the ambient temperature, H_0 and S_0 values are determined at this temperature. A number of definitions of exergy analysis exist, and in this study the following formula is used [20].

$$\eta_{EX} = \frac{EX_{produced}}{EX_{consumed}} \quad (6)$$

4.3. Shortcut V_{min} method

Engelien and Skogested [21] presented a shortcut method for comparing direct and indirect sequences. In this approach, the total amount of steam generated in each column is added up and compared for different processes. The sequence with the least amount of total steam will have the most efficient energy consumption. Eq. (7) provides the minimum steam rate in direct sequence.

$$V_{min}^{D} = V_{min}^{D,Col1} + V_{min}^{D,Col2} \quad (7)$$

Where V_{min} for the first and second column is calculated using Eq. (8) and (9), respectively.

$$V_{min}^{D,Col1} = \frac{\alpha_{AC} Z_A F}{\alpha_{AC} - \theta_A} \quad (8)$$

$$V_{min}^{D,Col2} = \frac{F(Z_B + Z_C)}{\alpha_{BC} - 1} + Z_B F \quad (9)$$

where F is feed flow rate, Z_i is mole fraction of component i in feed, and α_{iH} is volatility of component i relative to heavy component. θ is also the root of underwood equation which is determined using Eq. (10)

$$1 - q = \sum_{i=1}^{N} \frac{\alpha_{iH} Z_i}{\alpha_{iH} - \theta} \quad (10)$$

where q is liquid phase fraction in feed stream. In a ternary mixture, there are two possible calculated values for θ which satisfy Eq. (11).

$$\alpha_{AC} \succ \theta_A \succ \alpha_{BC} \succ \theta_B \succ \alpha_{CC} \ , \quad \alpha_{CC} = 1 \quad (11)$$

Eq. (12) illustrates α_i:

$$\alpha_{iH} = \frac{\left(\frac{y}{x}\right)_i}{\left(\frac{y}{x}\right)_H} = \frac{P_i^{sat}}{P_H^{sat}} \tag{12}$$

P_i^{sat} is vapor pressure of component i which is determined using antoine equation [22]:

$$\mathrm{Ln}P_i^{sat}\left[\mathrm{kPa}\right] = A - \frac{B}{T\left[^{\circ}C\right] + C} \tag{13}$$

Table 2. shows the values of A, B, C for three components of n-pentane, n-hexane, n-heptane.

Table 2. Parameters for Antoine equation

Feed component	A	B	C
n-pentane	13.7667	2451.88	232.014
n-hexane	13.8193	2696.04	224.317
n-heptane	13.8622	2910.26	216.432

The minimum steam rate in indirect sequence is determined using Eq. (14).

$$V_{min}^{In} = V_{min}^{In,Col1} + V_{min}^{In,Col2} \tag{14}$$

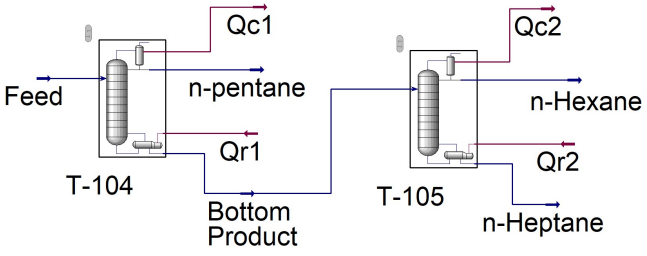
where V_{min} in the first and second column is calculated using Eq. (15) and (16), respectively.

$$V_{min}^{In,Col1} = \frac{\alpha_{AC} Z_A F}{\alpha_{AC} - \theta_B} + \frac{\alpha_{BC} Z_B F}{\alpha_{BC} - \theta_B} \tag{15}$$

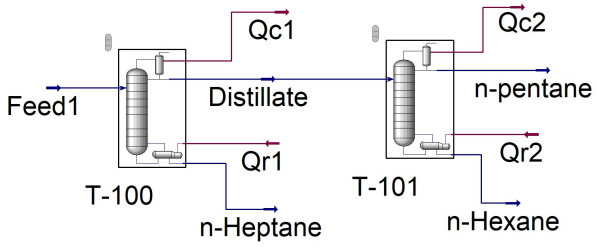
$$V_{min}^{In,Col2} = \frac{F(Z_A + Z_B)}{\alpha_{AB} - 1} + Z_A F \tag{16}$$

5. Results and discussion

This paper presents three different arrangements for separating the ternary mixture of n-pentane, n-hexane, and n-heptane. Fig. 1 illustrates direct and indirect sequence without heat integration simulations in Aspen HYSYS.



(a)

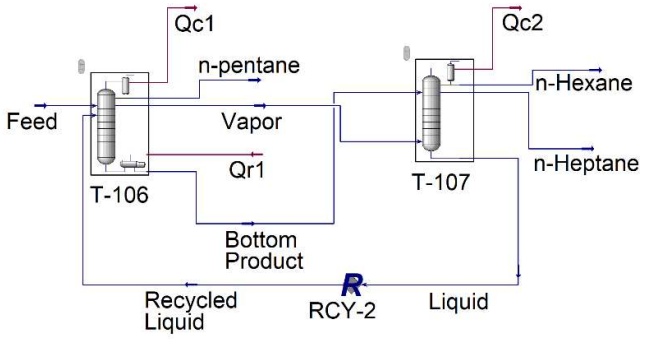


(b)

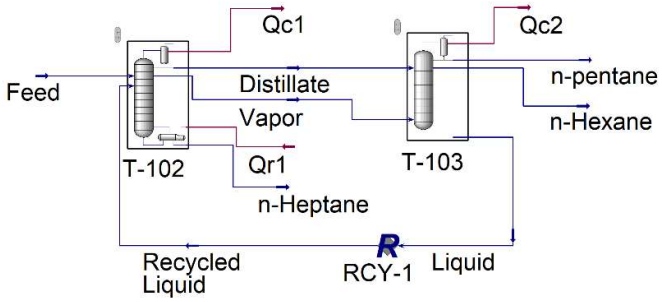
Fig. 1. (a) Direct sequence, (b) indirect sequence without heat integration

As shown in Fig. 1(a), the feed stream enters the first column through the 30th tray. This column has 52 trays. The distillate of the first column is pure n-heptane while the bottom products are n-pentane and n-hexane entering the second column from the 9th tray with the pressure of 430kPa and temperature of 96°C. This column involves 17 trays. The distillate and bottom product of this column are n-pentane and n-hexane, respectively.

In Fig. 1(b), the number of trays and the feed tray are similar to those in Fig. 1(a). There is, however, one major difference between these two processes, as the bottom product in the first column of Fig. 1(b) is pure n-pentene. The distillate consists of n-pentane and n-hexane introduced into the second distillation column under pressure of 430kPa and at a temperature of 96°C. N-pentane and n-hexane exit this column from the top and bottom, respectively. Fig. 2 also illustrates direct and indirect sequences with thermal coupling.



(a)

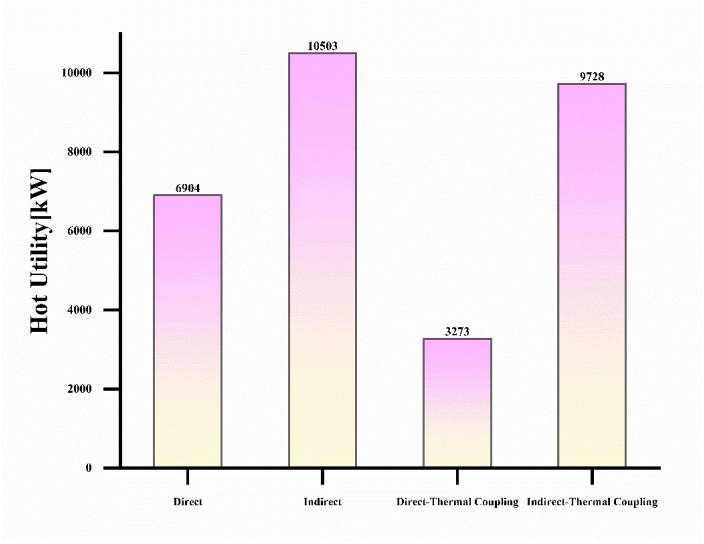


(b)

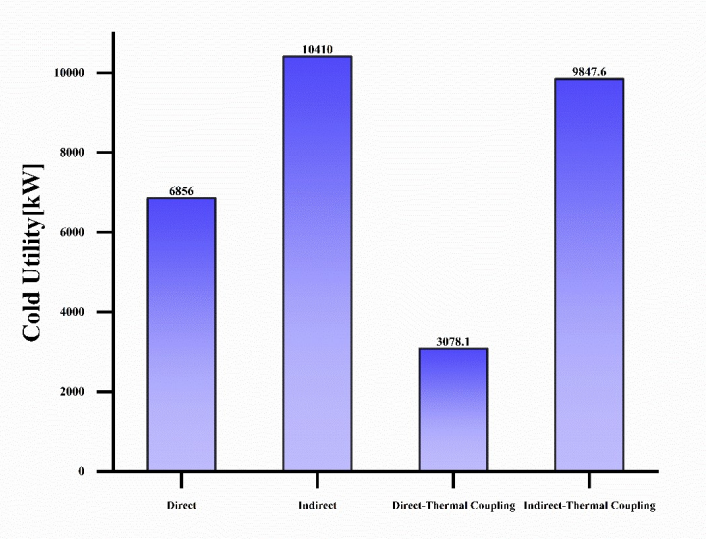
Fig. 2. (a) Direct sequence, (b) indirect sequence with thermal coupling

As indicated in Fig. 2(a), the feed stream enters the first column from the 30th tray. There are 52 trays in this column. N-pentane leaves the first column as the distillate, and n-hexane and n-heptane with a pressure of 450kPa and a temperature of 96°C, enter the second column from 6th tray as the bottom products. This 17-tray column does not have a reboiler. In the second column, n-pentane is the distillate, and n-hexane leave the 14th tray as the side stream. Through a vapor stream that exits the 51th tray of the first column and enters the bottom of the second column, the first column supplies steam to the second column. The second column bottom liquid product is returned to the 51th tray of the first column. This approach eliminates the distillation column's reboiler and as a result reduces the need for utility.

As indicated in Fig. 2(b), the feed stream enters the first column from the 30th tray. There are 52 trays in this column. N-heptane leaves the first column as the distillate, and n-hexane and n-pentane with a pressure of 450kPa and a temperature of 110°C, enter the second column from 9th tray as the bottom products. This 17-tray column does not have a reboiler. In the second column, n-pentane is the distillate, and n-hexane leave the 16th tray as the side stream. Through a vapor stream that exits the 3th tray of the first column and enters the bottom of the second column, the first column supplies steam to the second column. The second column bottom liquid product is returned to the 3th tray of the first column. This approach eliminates the distillation column's reboiler and as a result reduces the need for utility. Fig. 3 illustrates the comparison of cold and hot utility consumption for each of the four arrangements.



(a)



(b)

Fig. 3. (a) Hot utility, (b) cold utility for four processes

According to Fig. 3, the proposed direct sequence with thermal coupling decreases the hot and cold utility consumption significantly. Compared to indirect sequence, direct sequence reduces hot and cold consumption by 69% and 70%. Furthermore, Fig. 3 indicates that direct sequence in comparison to indirect sequence performs more efficiently. As a result, this sequence reduces the hot and cold utility consumption by 35% and 34% respectively,

compared with the indirect sequence. The simulation results are then compared with those obtained using the shortcut method. Fig. 4 demonstrates V_{min} for direct and indirect sequences.

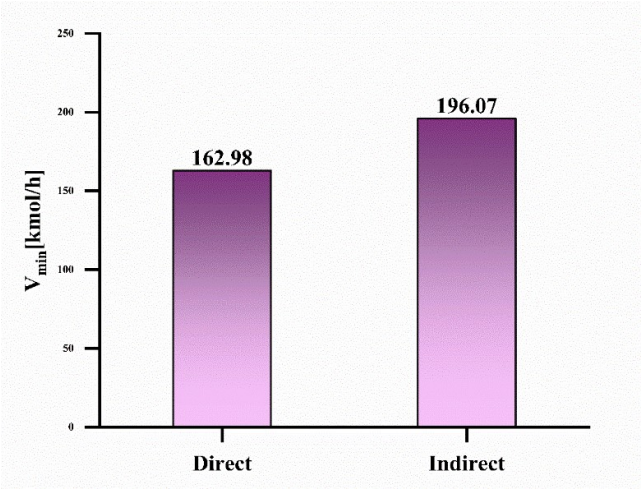
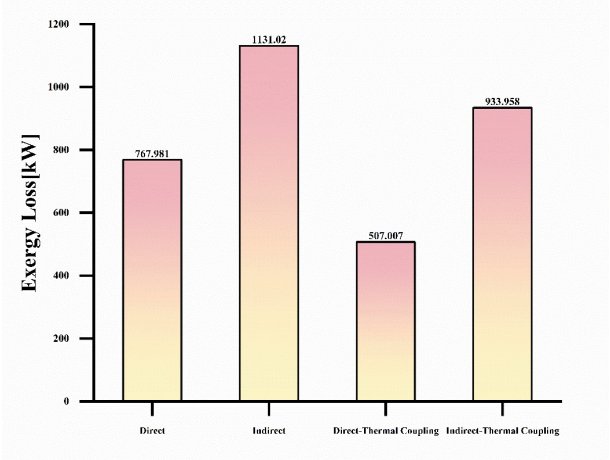
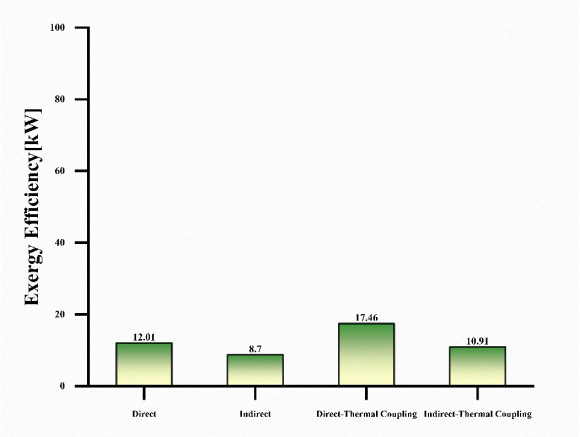


Fig. 4. V_{min} values for direct and indirect processes

As shown in Fig. 4, direct sequences provide superior performance to indirect sequences. It is evident from Fig. 3 and Fig. 4 that simulation results are in agreement with shortcut results. Fig. 5 illustrates the exergy loss and efficiency in different processes. In exergy calculations, ambient temperature (T_0) is assumed to be 25°C.



(a)



(b)

Fig. 5. (a) Exergy loss, (b) exergy efficiency for four processes

As shown in Fig. 5, the proposed direct with thermal coupling method provides the lowest exergy loss and the highest exergy efficiency. As compared to indirect sequence without heat integration, direct sequence results in a 55% reduction in exergy loss and a 9% increase in exergy efficiency. The figure also indicates that direct sequence reduces the exergy analysis and improves the exergy efficiency by 32% and 5%, respectively, when compared to indirect sequence. These results are in agreement with those obtained from simulation and shortcut V_{min}.

Table 3. Comparison between the results of the processes

Parameter	Direct	Indirect	Direct-Thermal coupling	Indirect-Thermal coupling
Hot utility reduction (%)	34.26	0	68.83	7.37
Cold utility reduction (%)	34.14	0	70.43	5.40
Exergy loss reduction (%)	32.09	0	55.17	17.42
Exergy efficiency increment (%)	3.31	0	8.76	2.21

6. Conclusion

There are two classical arrangements, direct and indirect for separating a ternary mixture of n-pentane, n-hexane, and n-heptane. In this paper, thermal coupling is proposed as a method of heat integration. All four processes are simulated using Aspen HYSYS. Energy analysis is integrated with exergy analysis in order to provide more accurate evaluation. Additionally, results from simulation of direct and indirect processes are compared with those obtained using the V_{min} shortcut method. In this paper, the following results are obtained:

1. Direct thermal coupling, as the proposed method in this study, is found to be the most efficient separation process. Comparing with indirect process without heat integration, Direct thermal coupling reduces energy consumption, exergy loss by 69% and 55% respectively, whereas the exergy efficacy is improved by 9%.
2. the effectiveness of direct thermal coupling process is attributed to the removal of the second column reboiler and considerable reduction in the heat load of the condenser.
3. In addition to cutting down on hot and cold utility usage (due to eliminating the reboiler in the second column), thermal coupling reduces TAC. Due to its ability to reduce hot and cold energy consumption considerably, this approach is also more environmentally sustainable.
4. All analysis, including energy analysis, exergy analysis, and V_{min}, clearly demonstrate the efficiency of direct processes over indirect processes. Additionally, using this sequence reduces energy consumption, exergy loss, and V_{min} by 34%, 32%, and 17%, respectively.

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