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PART B

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Design and Optimization of Intensified Quaternary Petlyuk Configuration

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Abstract

From its first introduction in 1965, the Petlyuk column received a high interest in the research community. Applied for the separation of three-component mixtures, the Petlyuk column is able to perform the separation with a reduced number of equipment and with a consistent reduction of the energy consumption compared to the classical sequences with simple columns. For a three-component separation the Petlyuk arrangement is composed by a prefractionator fully coupled with a main column that performs the separation of the products. Considering the great potential of these sequences it is natural to think about a possible extension to more than three component separations. In the present work a four component case is examined. If the divided wall column configuration is considered, the presence of three walls inside the main column makes the design and the control too complex to attract the industrial interest for a real application. New intensified sequences were proposed for the separation of four-component mixtures. These configurations use a less number of columns compared to the Petlyuk configuration. The case study reported proves the potential of the alternative configurations.

Keywords: Petlyuk configuration, distillation sequencing, design, energy saving.

1. Introduction

Two milestones are recognized by the research community as meaningful improvements in separations performed by distillation. The former is the introduction of structures with a partition wall inside the shell and the latter can be considered the definition of the Petlyuk configuration. Both of them were introduced almost fifty years ago but only recently have been successfully applied into the industrial practice for a limited number of feed components. Considering three-component separations, the Petlyuk configuration is composed by a prefractionator connected by two thermal couplings to the main column where the three products are obtained. If the prefractionator is included in the main column, the corresponding divided wall column (DWC) configuration is obtained. In both cases only one condenser and one reboiler are employed. It was clearly demonstrated that for a three-component mixture the Petlyuk configuration can

save up to 30 % of the energy consumption compare to the classical separation sequences (Emtir et al, 1999). Despite this evidence at least three valid hurdles contributed in the late development of Petlyuk and DWC configurations in the industrial practice. The first is the absence of recognized design methods, the second is the complexity of the structure and the third reason is the difficult in the process control. The research efforts, focused around these three points, contributed to reach more than one hundred operative DWCs around the world.
It is possible to assert that for the case of three component separations the Petlyuk and its equivalent DWC configuration has the potential of a noteworthy energy saving, different design methods are available, structure complexity are overcame by using the thermodynamically equivalent configurations and moreover the control issues are solved. It is clear that the same results are aimed for different number of feed components. Moving from three to four components the complexity of the Petlyuk and DWC structure increases and up to now only few studies are focused on the possible applications of these configurations. The aim of the present work is to propose alternative configurations to the Petlyuk/DWC configuration for a four-component separation. The benefit of the alternatives proposed is a simple design with a less or comparable total annual cost compare to the corresponding Petlyuk/DWC configuration. A case study is presented to support the new sequences.

2. Synthesis Procedure

The synthesis procedure is a systematic methodology that allows the prediction of all the alternatives generable from a sequence chosen as a reference. For a four-component mixture, the non-sharp configuration reported in Figure 1 is considered to start the generation procedure.

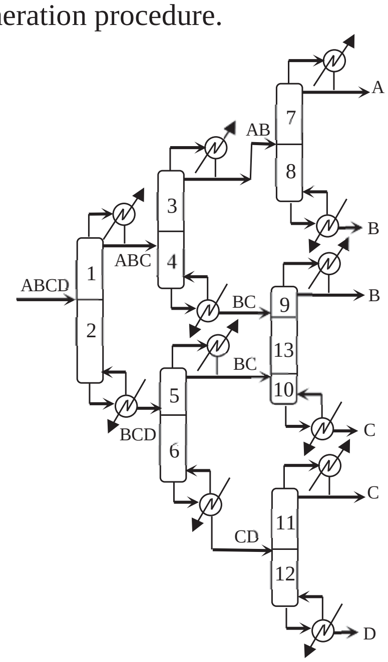

Figure 1. The six-column sequence for the fully sloppy separation of a quaternary mixture.

In this six-column sequence, usually referred as fully sloppy configuration, all the mixtures with three or more components are separated by symmetric sloppy splits. The corresponding Petlyuk configuration can be obtained in two steps: in the first one the column sections where the same mixture or component is separated are merged. In the case considered sections 4 and 5, 8 and 9, 10 and 11 are combined reducing the number of column to three. Then, considering that in the Petlyuk configuration there is only one condenser and one reboiler independently from the number of component to be separated, all the condensers and reboilers associated to non-product streams can be substituted with a thermal coupling. The corresponding configuration is showed in Figure 2.

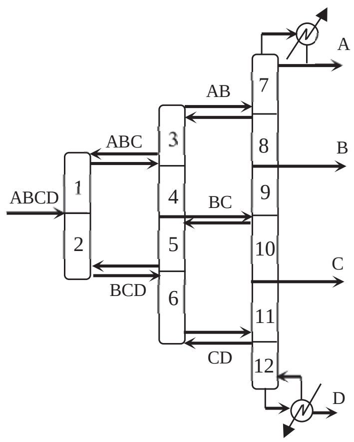

Figure 2: quaternary Petlyuk configuration

The Petlyuk configuration has three columns and five thermal couplings. Intensified sequences alternative to the Petlyuk arrangement can be obtained starting from the fully sloppy configuration of Figure 1 applying four different strategies (Rong at al, 2014):

1. Closed-Heat-Integration strategy to combine individual columns. This strategy is used to combine two columns by heat integration between a condenser and a reboiler co-producing a same product. This will reduce the number of columns.
2. Thermal coupling strategy to eliminate a condenser or a reboiler. This strategy is used to eliminate a condenser or a reboiler associated to a mixture of two or more components. This will reduce the number of heat exchangers.
3. Rearrangement of column sections strategy to generate thermodynamically equivalent structures. This strategy is used to recombine the column sections in a thermally coupled configuration through movement of the movable column sections. This will generate the thermodynamically equivalent structures which have different columns than the original thermally coupled configuration.
4. Elimination of the single-section-side columns strategy to produce the intensified distillation systems. For a thermally coupled configuration, there are thermodynamically equivalent structures in which there are single-section-side columns. This strategy is used to eliminate the single-section-side columns to generate the intensified distillation systems with fewer columns.

Applying the four point strategy presented the five configurations reported in Figure 3 are obtained. In particular the configuration reported in Figure 3(a) is obtained applying the strategy 1 to merge section 8 with section 9 and section 10 with section 11, then following the strategy 2 the condenser associated to the submixture ABC and the reboiler associated to the submixture BCD are substituted by thermal couplings. Strategy 3 is used to rearrange section 3 above section 1 and section 6 below section 2, finally single sections 4 and 5 are eliminated as indicated in the strategy 4. Similarly the configurations reported in Figure 3 (b-e) are obtained. Analyzing all the configurations generated is possible to notice that are all composed by two columns, moreover in sequences 3(b) and 3(d) the stream C is obtained twice, in sequences 3(c) and 3(e) the component B is recovered in two separate streams. Only the sequence 3(a) is associated to the minimum number of streams.

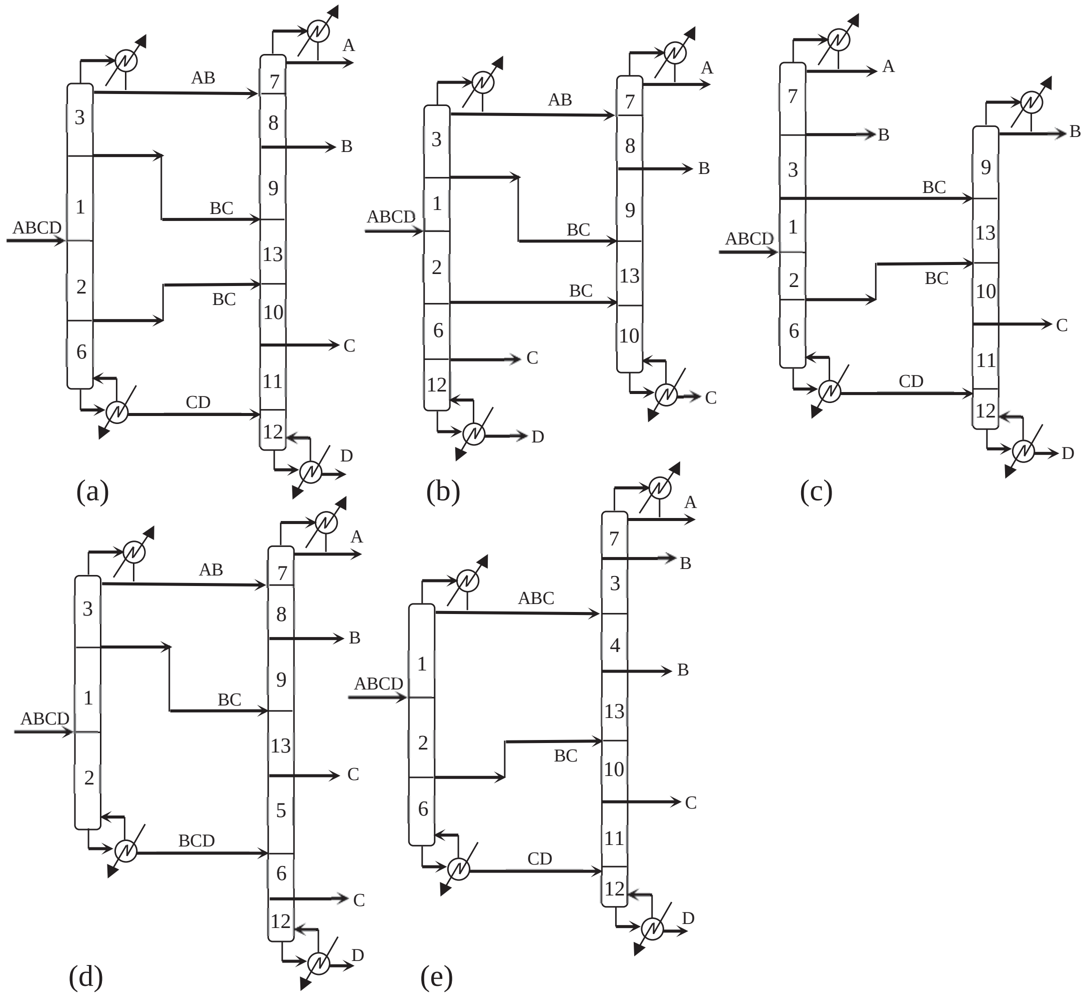

Figure 3: The intensified distillation alternatives for quaternary Petlyuk configuration

3. Case Study and Comparison Indexes

To test the applicability of the new intensified sequences, a case study has been considered. The composition and the product purity targets are shown in Table 1.

Table 1: feed composition and purity target

	Component	Feed composition [mol frac.]	Purity target [mol frac]
A	Butane	0.05	0.990
B	Hexane	0.10	0.970
C	Heptane	0.10	0.974
D	Nonane	0.75	0.997

A saturated liquid feed flowrate of 100 kmol h^{-1} is considered. All the configurations were simulated by means of Aspen Plus V8.0. The NRTL thermodynamic method was used and sieve trays columns were considered. The column pressure was optimized for

each column considering the possibility to use water in the condenser. The minimum temperature for the columns overhead vapor was defined to 323K.
Three different indexes were selected for the configurations comparison: the total annual cost, the thermodynamic efficiency and the carbon dioxide emission. The Total Annual Cost (TAC) is obtained as a sum of the operative and the annualized capital costs as reported in Eq. (1).

$$TAC = \sum \left[\left(\frac{Capital\ Cost}{Time\ of\ Investment} \right) + (Operative\ Costs) \right] \quad (1)$$

The operative costs were evaluated taking into account the cost of the water and the vapor in the condenser and reboiler respectively. The costs of the auxiliary fluids were obtained from Rev et al., 2001. The capital costs were considered as the sum of the costs of the condensers, reboilers, column shell and trays, evaluated according to the Guthrie's method reported in Turton et al., 2004. A mean investment time of 10 years was used to annualize the capital costs. The second index considered is how efficient the energy is being used. This information is expressed by the thermodynamic efficiency (η) evaluated as reported by Seader et al., 2009 and defined in Eq. (2)

$$\eta = -W_{min}/(-LW - W_{min}) \quad (2)$$

where W_{min} is the minimum work of separation and LW the lost work.
The last index used to compare the different configurations is the carbon dioxide emission (m_{co2}) since as a greenhouse gas is directly related to the global warming. The amount of carbon dioxide emitted was evaluated by the Eq. (3) following the method reported by Gadalla et al., 2005:

$$m_{CO_2} = \left(\frac{Q_{FUEL}}{NHV} \right) \left(\frac{\%C}{100} \right) \alpha \quad (3)$$

where Q_{fuel} is the heat generated by the combustion reaction, NHV the net heating value of a fuel with a carbon content of %C and α the ratio of molar masses of CO_2.

4. Simulations and results

In order to get the design parameters of all the alternative sequences, the fully sloppy configuration of Figure 1 was first simulated using the short-cut method of Underwood-Gilliland-Winn already implemented in Aspen Plus. The parameters obtained were used to initialize the stage-to-stage rigorous method RadFrac. The number of stages, feed location, reflux ratio were then optimized for the minimum energy consumption.
The design of the Petlyuk configuration was performed considering the correspondent among the column sections functionality (Errico et al., 2014). In this way once the design of the fully sloppy configuration of Figure 1 was obtained the configuration parameters were transposed to the analogous sections. The thermal coupling the flowrates were defined as the minimum possible value to assure the products purity targets. Following the same design methodology cited for the Petlyuk configuration, the alternative configurations reported in Figure 3 have been simulated using the correspondence of column functionality. Only the results for the configuration of Figure 3(a) are reported in Table 2 since, for the composition cases considered, was most convenient from the energy consumption point of view. Among all the alternatives predicted, the one in Figure 3(a), is the only sequence that performs the separation of the middle components once.

Table 2: Sequences comparison

	Petlyuk	Fig. 3(a)
TAC [$/y]	433	432
η [%]	47	52
CO_2 [kg/h]	601	598

5. Conclusions

The work presented a new space of alternatives to the Petlyuk configuration for quaternary separation. The motivation of the work starts from the interest in the Petlyuk configuration due to its potential in energy reduction. Anyway for a four-component separation, the complexity of the design and control limit its application. A synthesis methodology is presented to generate a complete space of alternatives with a simpler design. For the case considered, among all the sequences it was obtained once with similar or better performance compare to the Petlyuk configuration. It is possible to conclude that the alternatives proposed are a valid alternative to the complexity of the Petlyuk configuration but still with the same benefit of less energy consumption.

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