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Grau en
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Treball Final de Grau

Comparison of Energy used by Side Columns and Conventional Columns for ternary mixture separation.

Comparació de l’energia utilitzada per les Columnes Convencionals i amb rectificadors laterals per la separació de mescles ternàries.

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BARCELONA

“The only source of knowledge is experience.”

Albert Einstien

En primer lloc vull agrair a la meva germana, mare i amics, especialment als que van estar atents i em van proporcionar la seva ajuda en els diferents avenços d'aquesta trajectòria sobretot en els moments mes difícils.

Als meus tutors que em van guiar a la finalització d'aquest projecte del grau.

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SUMMARY

Distillation is one of the most used unit operation in chemical industry, which is based on the separation of mixtures of two of more components based upon their respective boiling points. In a separation of an ideal ternary mixture two sharp splits distillation columns sequences are widely used, the direct one and the indirect one, but negative point of types of sequence are that they consume a lot of energy to make the desired separation possible.

In order to reduce the overall operational costs and make this separation energetically efficient, columns with side rectifiers and side strippers were proposed but unfortunately the advantages of this sort of columns is not clear from the published literature, therefore the use of these columns is very limited.

The basic aim of this work is the comparison between the amount of energy consumed in the separation of ideal ternary mixture by the conventional process schemes and the intensified columns with side columns, in order to find when the intensification could have a higher potential and advantages to be implemented. A rigorous simulation of three different types of ideal ternary mixtures is performed in Aspen with conventional and intensified methods to make a comparison between them.

Keywords: Side Columns

RESUM

La destil·lació és una de les operacions d'unitats més utilitzades en la indústria química que es basa en la separació de les barreges de dos components o més per la diferència entre els seus punts d'ebullició respectius. En la separació d'una mescla ternària ideal, actualment tenim present dues seqüències de columnes de destil·lació mes utilitzades, la directa i la indirecta En aquestes tipus de seqüències, les dues columnes consumeixen molta energia, per fer possible la separació desitjada.

Per tal de reduir els costos operatius i fer aquesta separació sigui eficient i gasti menys energia, es van inventar columnes amb strippers laterals i rectificadors laterals, però malauradament no s'han fet moltes investigacions sobre aquestes columnes, pertant las seves utilitzacions en la industria son molt limitada.

L'objectiu bàsic d'aquest treball serà la comparació de la quantitat d'energia consumida en la separació de la barreja ternària ideal pels mètodes convencionals i les columnes d'eficiència energètica amb rectificadors laterals, per tal de trobar quina és millor. En AspenPlus 10 es farà una simulació rigorosa de tres mescles ternàries ideals diferents amb columnes convencional i columnes laterals.

Paraules Clau: Columnes Laterals

1. INTRODUCTION

Distillation is one of the most important, oldest and widely used key separation unit operation of the chemical industry. The operational costs associated to carry out this operation are also very high as lot of energy is inverted in this process to make the distillation columns function. Therefore, the optimization of this process has remained as one of the key aspects in the past and a lot of research is still being carried out till date to make this process more energetically efficient.

Many studies conducted by different authors suggested the use of side columns (columns with side rectifiers and side strippers) for this process as being one of the best solution for this problem as significant amount of energy reductions can be obtained with these configurations, but some others studies has also revealed that the use of these types of columns didn’t proved to be as effective in reducing the operational costs apart from generating additional installation costs. Therefore, it is not very clear yet if the use of these types of columns can be energetically efficient and if so in which of those cases

The reason behind the lot of research that has been carried out is because the operational cost of these processes is very high and can consumes about 40-60% of the total energy used in the industry. In other words, the use of lots of energy producing resources which contributes a lot in the deterioration of the environment.

In a study carried out by Tedder and Rudd (1978), it was found that the complex distillation sequences such as side strippers or rectifiers may offer significant energy savings over conventional sharp split distillation sequences for ternary mixture. The research on these columns were intensified by Triantafyllou and Smith (1992), when they started the designing and optimization of these thermally coupled columns.

Promising results were obtained by Flores (2003) when a significant amount of savings of around 10% to 26% were achieved in the separation of mixture of alkanes, depending on different concentration of components present. But Wang (2018) simulated several ideal ternary mixtures of alkanes from 4 to 8 carbons i and found that the direct sequence with backward energy integration consumes less energy than the side-rectifier and that the side stripper.

Although the authors mentioned above arrived at different conclusions based on the results obtained, but there were still studies conducted on these columns which were never compared with the results that could have been obtained with the conventional columns.

Moreover, other studies conducted by authors like Wang (2013), Nikolae (2017) and Tarjani (2018) suggests that the conventional columns used in separation processes for ideal ternary mixture were more energetically efficient with respect to side columns, as a result of what the attention on side columns as a possible good alternative for ideal mixtures was deviated to non-ideal mixtures. For example, the use of extractive distillation.

Therefore, to prove the effectiveness of these columns more strong and detailed evidence are needed.

1.1. CONVENTIONAL DISTILLATION COLUMNS

The conventional columns are the one widely used in the chemical industry for the purpose of distillation. These columns are basically equipped with one reboiler at the bottom, which is used to provide the energy necessary to boil the mixture and make the column work and the head is connected with a partial or total condenser to condensate the vapor obtained. When the mixture of two components is introduced to the column, the component which has the lowest boiling temperature is evaporated from the heaviest component along with some impurities of heavy component and tends to go up and is recovered at the head of the column. The vapor obtained is then passed though the condenser for phase change and is obtained it in its liquid form which is known as distillate. The distillate recovered at the top is never 100% pure because certain impurities of the other component are present and the residue from the bottom is also obtained with certain impurities of light component.

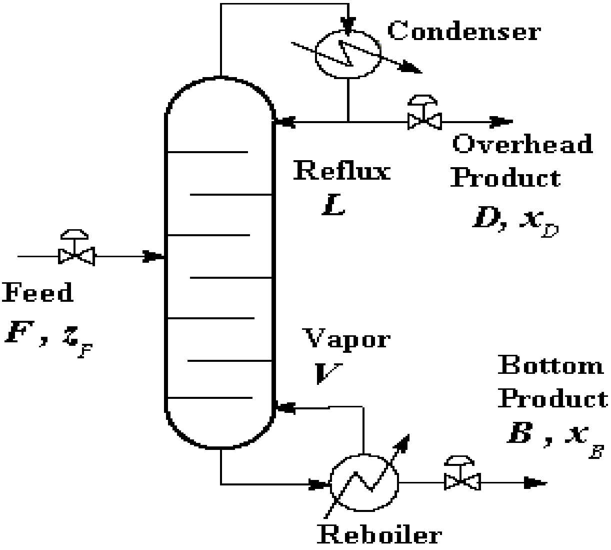

Figure 1: Distillation column

1.2. DIFFERENT SEQUENCES

For the separation of binary mixture, only one distillation column is sufficient as both products can be separated and obtained from the top and bottom of the columns, but if the mixture consists of more than two components then more distillation columns are required for the separation process. To connect these columns in series, different types of sequences are available depending on the properties of components of the mixture.

1.2.1. Direct Sequence

Direct sequence is used when there is a significant difference in the boiling points of lightest component with respect to other two components in the mixture and the lightest component is the first one to be separated.

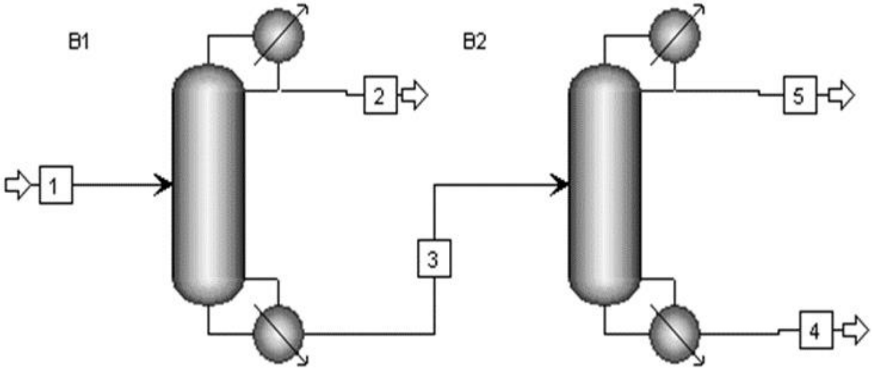

Figure 2 Distillation columns connected in direct sequence

A ternary mixture is introduced to the first column (C1) where the first separation takes place. The lightest component enriched vapor with certain impurities is collected from the head of the C1 and the resultant mixture of the other two components, which is collected at the bottom of the first column serves as the feed for the next column (C2) where the second separation process take place. Once again, a vapor enriched in intermediate component with certain impurities of other components is obtained at the head of the C2 and the heaviest one of all is obtained from the bottom of C2.

The number of columns which must be connected in series depends on the number of components present in the feed stream. For example, if the stream consists of four components then a configuration of 3 columns is required.

1.2.2. Indirect Sequence

As the name suggests the functioning of indirect sequence is totally inverse with respect to direct sequence, as the difference between boiling point of the heavy component with respect to other two components is significantly higher, which implies the separation of heavy component from the other two much easier. Therefore, our priority is to separate the heavy component.

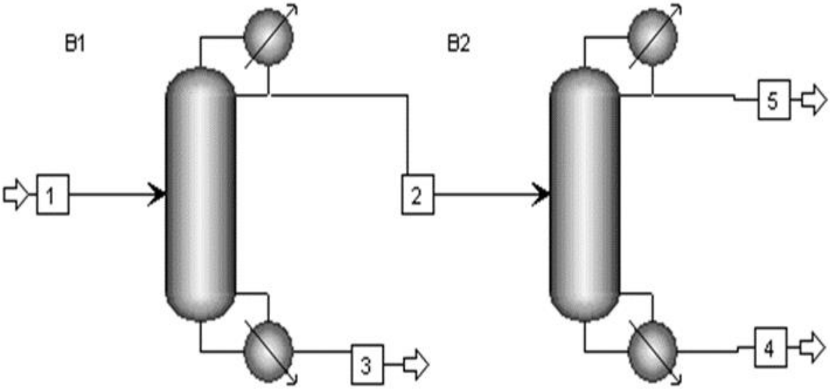

Figure 3 Distillation columns connected in indirect sequence

A ternary mixture is introduced to the first column (C1) where heaviest component is separated from the other two components and is recovered from the bottom of C1. The vapor which is obtained from the top of the column is a product of other two components with certain impurities of the heavy component, is sent to the second column (C2) for the second separation. Vapor enriched in the lightest component is obtained from the top of C2 and residue with intermediate component is collected from the bottom.

1.2.3. Side Columns

Side columns are also used to separate the ternary mixtures but, in this separation, there is only one main distillation column which is integrated with a side rectifier o side stripper as shown in figure 4.

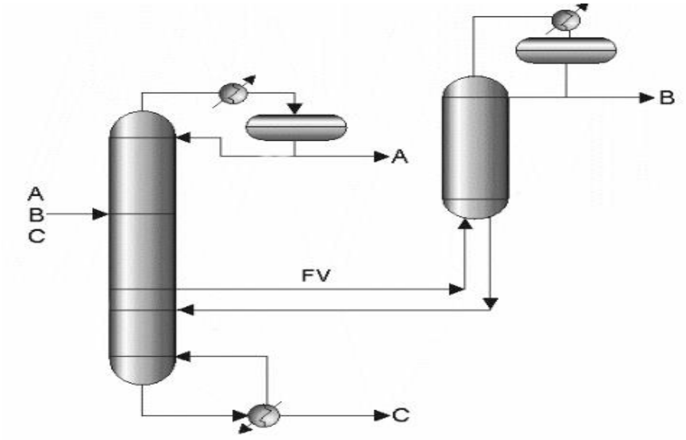

Figure 4 Distillation column with side rectifier

As usual the ternary mixture is added to the main column (C1) where the distillation process takes place. When the mixture is boiled the component, whose boiling temperature is lower than other two components tend to evaporate with certain impurities and a vapor enriched with lightest component is collected at the top. But as we descend in the column, every time the vapor resultant is more enriched in intermediate component and heavier component rather than the lighter one. To take advantage of this vapor highly enriched in intermediate component, a side rectifier (C2) is connected to the main column where that intermediate component enriched vapor extracted laterally from the C1 is introduced. In this side rectifier C2, the second separation takes place. Intermediate component which has a lower boiling point remain in the vapor form and is collected form the head of the side rectifier, whereas the heavy component which has higher boiling point starts to condensate and is returned to the main column C1, where it keeps on concentrating and finally is recovered from the bottom of the main column. In this way the energy which was used previously by reboiler of the second column in the conventional configuration is saved.

2. OBJECTIVES

The main objective of this work is to find out in which cases the use of side columns is more efficient than the conventional columns. Rigorous simulations will be done in the AspenPlus 10 and the results obtained will be compared to find out which one is the best.

The results obtained with rigorous simulations will also be compared with the results obtained in the studies of all other authors to prove the validation and effectiveness of those studies for these types of columns.

3. METHODOLOGY

In this section a brief explanation has been given on the methodology used to carry out the simulation procedure. The simulation program used in this work was Aspen Plus v.10 and the thermodynamic models used in each simulation were different because the thermodynamic behaviour of every ternary mixture is different and depends much on the physical and chemical properties of components present.

During the simulation, large number of plates were implemented in each column section to determine a value close to the minimum amount of energy required. The optimum reflux ratio used for simulation was calculated based on the distillation heuristic which states that, optimum reflux ratio must be around 20% more than the minimum reflux ratio. If the reflux ratio calculated is not being around its optimum It is still not a big problem as just being around its optimal point it can still give us a good measure of the potential savings of each process.

A mixture of 100 kmol/h was selected for the simulation process, and the amount of heavy compound present in the intermediate product stream was set to 10 kmol/h and the purity of all products to 99.9% to make the comparison. As the composition of the feed influences the energy consumption, a sensitivity analysis was performed by fluctuating the flow of intermediate and light component while the flow rate of heavy component remained constant.

The optimization of the process was done in cases where a significant potential energy saving was detected.

4. TERNARY MIXTURES SELECTION

The selection of all thee mixtures was made based on different studies conducted by several authors in which significant amount of energy savings were obtained as mentioned above.

A mixture of pentane, hexane and decane was selected based on the simulations conducted by Flores in case of alkanes mixture in which energy savings varying from 10% to 26% depending on the mixture and the proportion of compounds was obtained.

The second mixture selected was the mixture of alcohols which was composed of methanol, ethanol and hexanol. The selection of this mixture was based on the simulation conducted by Tarjani (2018) in which he proved that the conventional distillation is more energetically efficient than the use of side rectifiers in distillation of alcohols mixture.

The third and the last mixture that was selected was the mixture of aromatics components composed of heptane, toluene and aniline. This mixture was selected because of simulations conducted by Sun (2014) for aromatic mixture in which he achieved an overall energy saving of 22% with the side stripper

4.1. SIMULATION OF DIFFERENT MIXTURES

The simulation conditions for all three different mixtures that were simulated are described below:

4.1.1. Mixture of pentane, hexane and decane

This ternary mixture is a typical product of the petrochemical industry. The mixtures basically consist of two alkanes pentane and hexane with nearer boiling temperature of 36.1ºC and 68ºC respectively and decane with a boiling temperature of 174.1ºC which is quite higher than the other two.

- Simulation conditions:

Table 1: Simulation conditions for Alkanes mixture

Temperature of columns (ºC)	25
Pressure of columns (atm)	1
Thermodynamic model	PRBM
Feed (kmol/h)	100

The columns used in this simulation were working at a fix temperature of 25ºC and at a constant pressure of 1 atm. The thermodynamic method used for this mixture was of Peng-Robinson equation of state with the Boston Mathias modification (PRBM). A constant mixture of 100 kmol/h was continuously feed to the column with molar fraction indicated in table 2.

Table 2: Molar composition of Alkanes mixture

component	Mole fraction (%)
pentane	80
hexane	10
decane	10

4.1.2. Mixture of methanol, ethanol and hexanol

This mixture basically is composed of three different types of alcohols. Two of these alcohols, methanol and hexanol have relatively closed boiling temperatures of 64.7ºC and 78.4ºC, whereas the boiling temperature of hexanol is 157ºC way higher than the other two.

- Simulation conditions.

Table 3: Simulation conditions for Alcohols mixture

Temperature of columns (ºC)	25
Pressure of columns (atm)	1
Thermodynamic method	UNIQUAC
Feed (kmol/h)	100

The columns used in this simulation were working at a constant temperature of 25ºC and a fixed pressure of 1 atm. A constant feed of 100 kmol/h was introduced in the distillation column, but the thermodynamic model used in this simulation was UNIQUAC, as this model is widely used for the mixtures of alcohols.

The molar composition of the feed inserted is described in the table 4.

Table 4: Molar composition of Alcohols mixture

component	Mole fraction (%)
methanol	80
ethanol	10
hexanol	10

4.1.3. Mixture of heptane, toluene and aniline

The third mixture that was selected was made up of aromatic, aliphatic and naphthalic compounds known as heptane, toluene and aniline with respective boiling temperatures of 98.4ºC,110.6ºC and 184.1ºC. Like other two mixtures, the boiling points of the light and intermediate are very closer to each other and are very far away from the heavier component.

- Simulation conditions

Table 5: Simulation conditions for Aromatics mixture

Temperature of columns (ºC)	25
Pressure of columns (atm)	1
Thermodynamic method	UNIQUAC
Feed (kmol/h)	100

The columns used in the simulation of this mixture were also operating at a temperature of 25ºC and overall pressure of 1 atm. Like other two mixtures a constant flow of 100 kmol/h of the mixture was also feed to the column. The thermodynamic model used in the program was UNIQUAC.

The molar composition of the feed to the column is presented in table 6.

Table 5: Molar composition of Aromatics mixture

component	Mole fraction (%)
heptane	80
toluene	10
aniline	10

Once the simulation conditions were fixed, the simulation of these mixtures took place in number of different cases described in table7.

Table 7: Different cases proposed for simulation

Mixture	Cases	Variables	
		FFR (kmol/h)	HFR (kmol/h)
Alkanes	1	100	10
	2	100	20
	3	100	30
	4	100	40
	5	100	50
	6	100	60
	7	100	70
	8	120	10
Alcohols	1	100	10
	2	100	20
	3	100	30
	4	100	40
	5	100	50
	6	100	60
	7	100	70
Aromatics	1	100	10
	2	100	20
	3	100	30
	4	100	40
	5	100	50
	6	100	60
	7	100	70

- FFR - Feed flow rate
- HFR - Heavy component flow rate in the feed

In each mixture the variables that were manipulated were the total feed flow rate varying from 100 kmol/h to 120 kmol/h and the flow rate of heavy component in the feed from 10 to 70 kmol/h. Once these flow rates were fixed, a sensitivity analysis was conducted varying the flow rates of intermediate and light component.

After determining the simulation conditions the designing of the columns comes next. For the designing of direct sequence columns, the two factors that were taken into consideration were the purity of the product that we want to achieve from the top of the column and the reflux ratio.

Table 8: Design specifications of distillation columns 1 and 2 for direct sequence

Nº of plates	90
feed plate	45
reflux ratio	1.2 of reflux minim
product purity	0.999

In case of columns equipped with the side rectifiers the designing of the column was bit different than the direct sequence. For main distillation column (C1) same sort of conditions were taken into account like the 20% more of minimum reflux ratio and product purity of 99.9%, but in case of side rectifier (C2) as there is no reboiler present to change the vapor conditions and fix the product purity at the head, the only variable that was taken into account was the distillate flow rate. The distillate flow rates were calculated from the mass balances in Fortran and were exported to the distillate rate of each column using a Calculator. These distillate flow rates were calculated assuming that the impurity present in the light and heavy product streams was of the intermediate boiling compound. The overall design specification for the column with side rectifier are described below.

Table 9: Design specifications for distillation column equipped with side rectifier

Nº of plates	90
feed plate	45
lateral extraction plate	30
lateral insertion plate	60
reflux ratio	1.2 of reflux minim
product purity (C1)	0.999
product purity (C2)	0.999

5. RESULTS

The results obtained from the simulations of different cases proposed above are discussed in this section and non-converged simulations are discharged.

The results obtained for each mixture are describe below.

5.1. MIXTURE OF PENTANE, HEXANE AND DECANE:

After briefly analysing the results obtained from the mixture of alkanes present in table 10 which can be found in Appendix 1, we can observe that by fixing the flow rate of heavy component and keep varying the molar composition between intermediate and light component the energy consumption keeps on changing. The amount of energy used by both columns is lower when the amount of Lighter component in the feed is higher than the intermediate component, but as soon as the ratio of intermediate component tends to increase, so does the energy consumption.

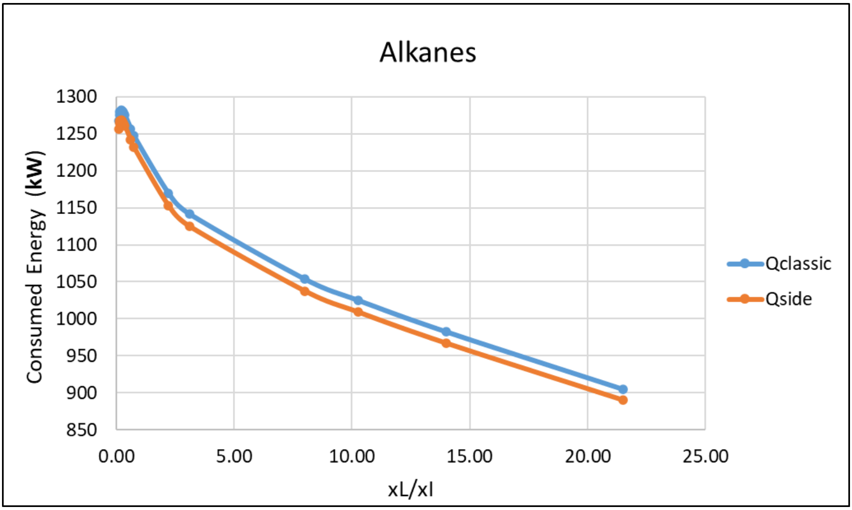

Figure 5 Energy consumed by conventional configuration and side rectifier

From figure 5 it is quite clear that when the quantity of lighter component in the feed is higher as compared to the intermediate component, columns with side rectifier use less energy than the conventional one's, but as soon as the ratio between the light and intermediate component keeps on decreasing, in other words the amount of intermediate component keeps on increasing and the difference between both curves of energies keeps on decreasing till these two becomes practically equals.

Although a difference in energy consumption has been observed in the figure 5 but it does not seem to be efficient as the two lines that marks the energy consumed for the two methods are relatively close to each other.

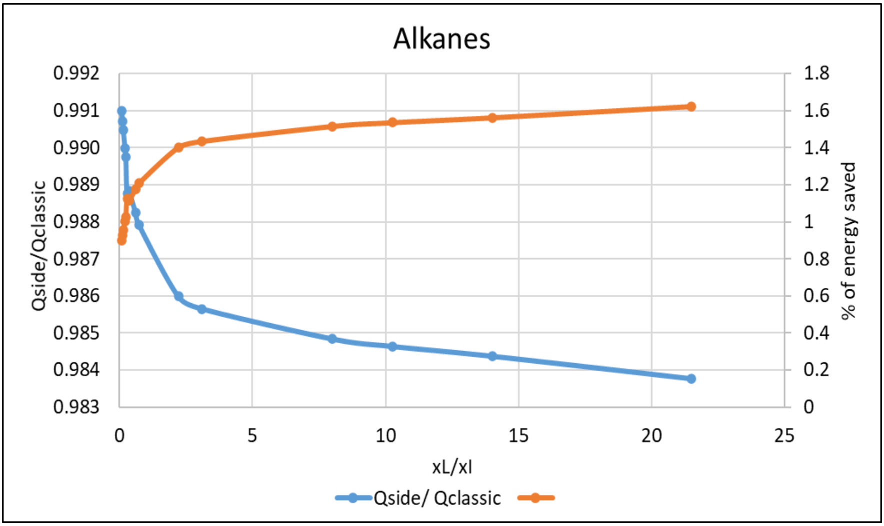

Figure 6 Ratio between Qside and Qclassic for Alkanes mixture

The effectiveness of side columns can also be explained figure 6, where the maximum amount of energy saved by the side rectifiers in best of the cases is approximately around 1.6% as compared to the conventional methods

After fixing the molar composition of heavy component to 10 kmol/h no significant differences were observed in case of energy saving, some more simulations were done by varying the flow rate of the heavy component from 20 kmol/h to 70 kmol/h. Same sort of sensitivity analysis was done for the intermediate and light component In these simulations, for different flow rates of the heavy component and the results obtained after the simulation are shown in figure 7. The simulation data for this figure can be found in Appendix 1.

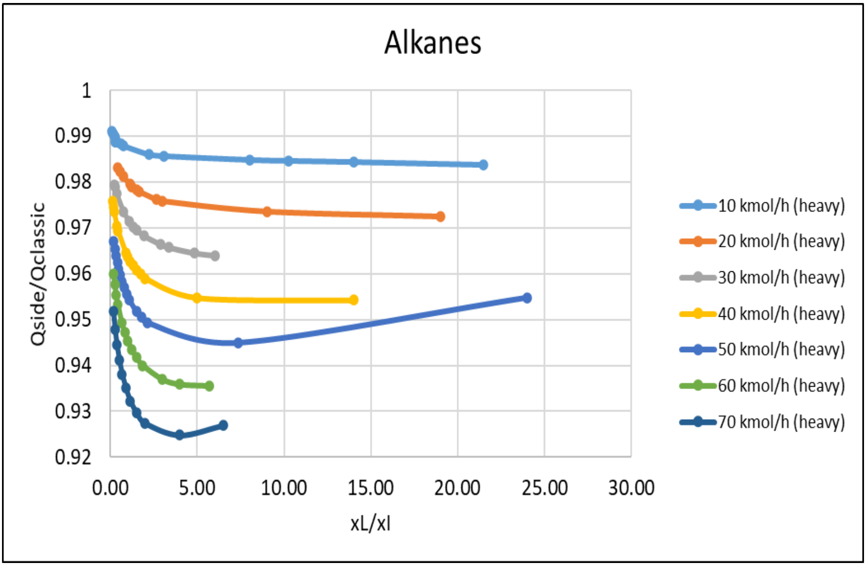

Figure 7: Ratio between Qside and Qclassic for Alkanes mixture for different flow rates of Heavy component in the feed.

It is quite clear form the figure 7 that as we keep on increasing the proportion of heavy component in the feed, the amount of energy consumed in the side rectifier keep on decreasing as compared to conventional distillation sequence. The more the amount of heavy component lesser is the energy consumed in the columns with side rectifiers as compared to conventional columns. Although it is quite evident from the figure, the trend that follows different simulations. For higher quantities of intermediate component in the feed the amount of energy used is larger and keeps on decreasing as the amount of lighter component keeps on increasing, but some unusual types of behaviours have also been marked for the flow rates of 50 kmol/h and 70 kmol/h of Heavy component. In the beginning for lower proportion of intermediate component with respect to lighter, the energy consumption by Qside rectifier is lower as compared to Q classic up to certain, but as we keep on increasing the amount of lighter component in the feed side rectifiers starts to consume more energy, which is quite extraordinary because when the amount of lighter component is increased the reboiler of the column has to provide less energy to boil the mixture

Another simulation of the same mixture was done by varying the overall feed rate from 100 kmol/h to 120 kmol/h to find out, how it affects the overall energy consumption and the results are described in the figure 8. The simulation results for this graphic can be found in Appendix 1.

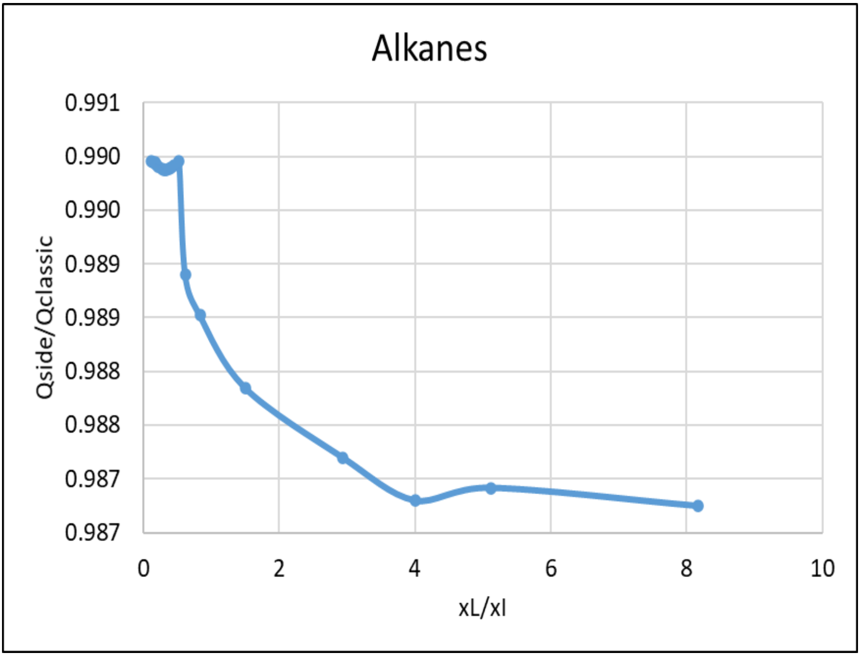

Figure 8: Ratio between Qside and Qclassic for Alkanes mixture with initial feed rate of 120 kmol/h

A similar sort of tendency can be observed in the mixture with initial feed rate of 120 kmol/h with respect to that of 100 kmol/h which is quite evident because at the end we are just changing the base of our calculations.

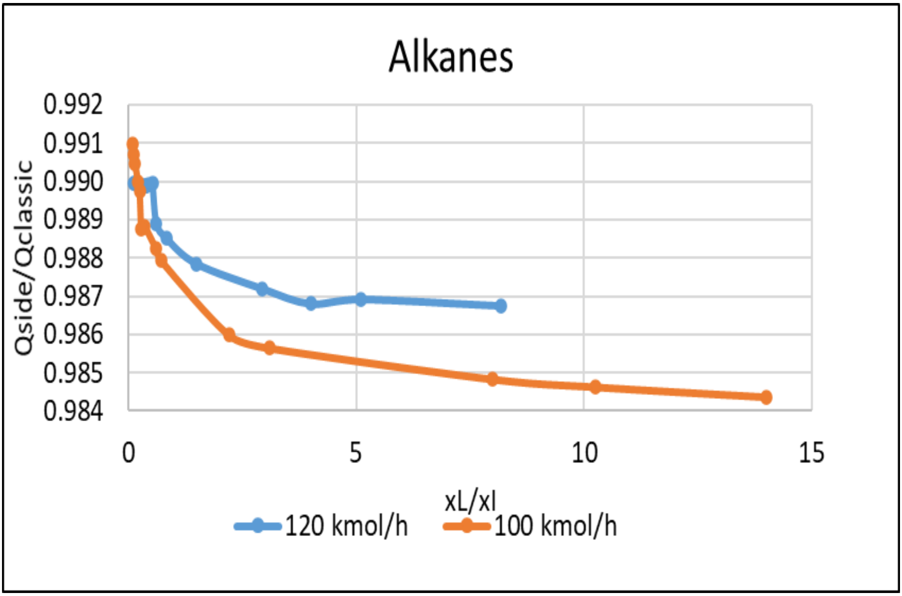

Figure 9: Comparison of energy consumption for Alkanes mixture with feed rate of 100 kmol/h and 120 kmol/h

When the energy consumption for two different feed rates indicated above were compared with each other in figure 9, clear differences were observed but they are not significant because they are affecting the third decimal of the ratio between Qside and Qclassic. This is because Aspen converges the numerical results with some established accuracy and therefore the third decimal of the ratio does not matter

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A further study was conducted by comparing the energy used by both configurations in their optimized mode (columns in which the number of plates has been reduced to optimum number) and non-optimized mode (columns in which large number of plates were used for the simulation).

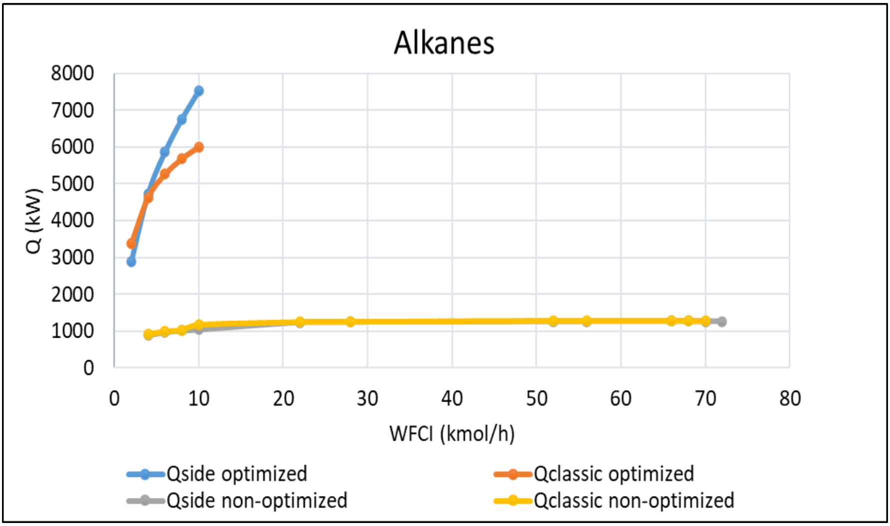

Figure 10: Comparison of energy consumption for Alkanes mixture with columns in optimized and non-optimized conditions.

It was found that for the higher flow rates of intermediate component in the feed, the energy consumed by side rectifier in optimized condition is way higher than the one used by conventional columns, but when the comparison is done between the optimized and non-optimized columns it is quite evident that the energy used by the optimized columns for the same feed composition is way higher than the one used by conventional columns. For the flow rate of 10 kmol/h of intermediate component, the energy used by Qside rectifier in optimized condition is around 7500 kW, whereas used by Qside rectifier in non-optimized condition is around 1100 kW.

5.2. MIXTURE OF METHANOL, ETHANOL AND HEXANOL

The results of sensitivity analysis conducted by AspenPlus for the simulation conditions described above for this mixture is represented in the figure 11 which is obtained from the simulations results present in Appendix2.

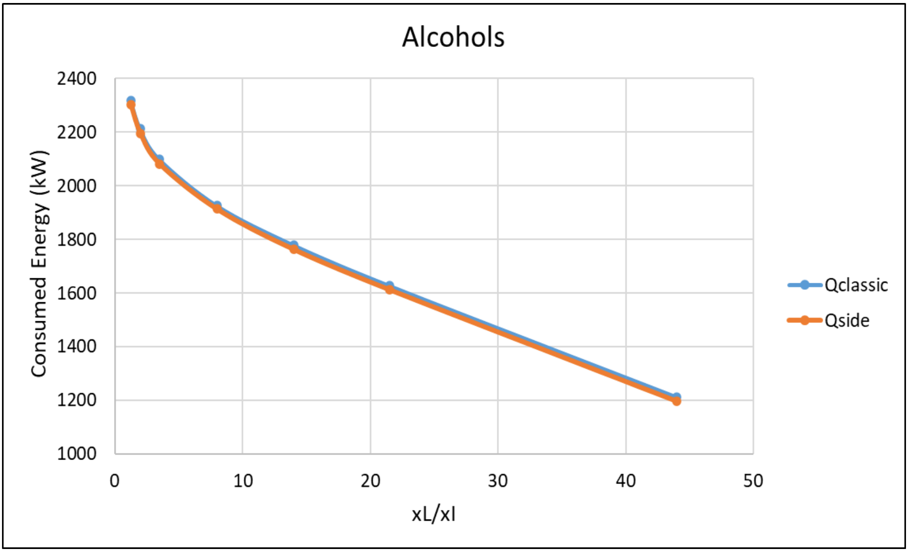

Figure11: Energy consumed by conventional configuration and side rectifier

By fixing the heavy component flow rate at 10 kmol/h and varying the proportion between light and intermediate feed (xL/xI) for the total feed rate of 100 kmol/h, it was observed form the figure 11 that the energy consumed by both configurations is practically identic for every proportion of intermediate and light component.

When the same mixture of alcohols is simulated but varying the feed rate of the heavy component like we did in the previous mixture, a same sort of trend can be seen in figure 12 as compared to the previous mixture. For higher flow rates of lighter component, a decrease in the consumption of energy is observed in the side rectifiers as compared to the conventional columns and the maximum savings of around 6% is detected in the case of flow rate with 60 kmol/h of the intermediate component. But apart from this, an abnormality in the curve has been observed for the flow rate of 10 and 20 kmol/h. According to the theory when we increase the flow rate of intermediate component, the xB ratio in the feed increases which results in more energy consumption to boil the mixture. The fraction between the Qside and Qclassic keeps on increasing for higher proportion of intermediate component as the energy consumed by the side rectifier increases and the overall proportion tends to 1. But In between a sudden rise in the consume of energy by side rectifier has been recorded for lower proportion of intermediate component as compared to one used by side rectifier for higher proportion of the same component. The simulation results corresponding to figure 12 can be found in Appendix2.

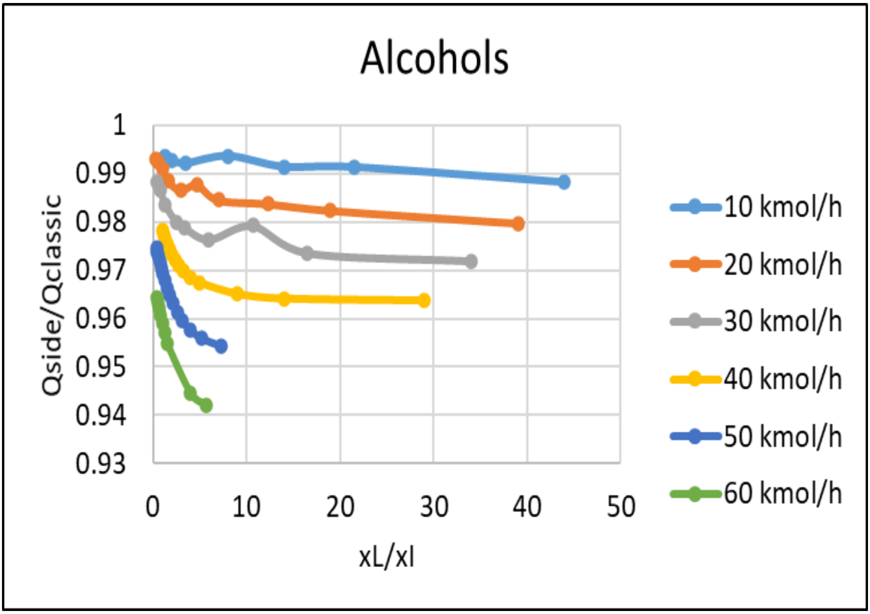

Figure 12: Ratio between Qside and Qclassic for Alkanes mixture for different flow rates of Heavy component in the feed.

5.3. MIXTURE OF HEPTANE, TOLUENE AND ANILINE

Results obtained for the mixture of aromatic component are quite different from the results obtained for the other two mixtures. In the previous two mixtures, the energy consumption by both configurations was increased as the flow rate of the intermediate component was increased, but in this case a different type of curve is observed in figure 13. For the overall flow rate of 100 kmol/h and with fixed flow rate of the heavy component of the 10 kmol/h, when the flow rate of intermediate component in the mixture starts to increase so does the energy consumption by both configurations but up to certain extent and then for further increase in the flow rate the energy consumption starts to decrease. In Appenix 3, the simulation results of figure 13 can be found.

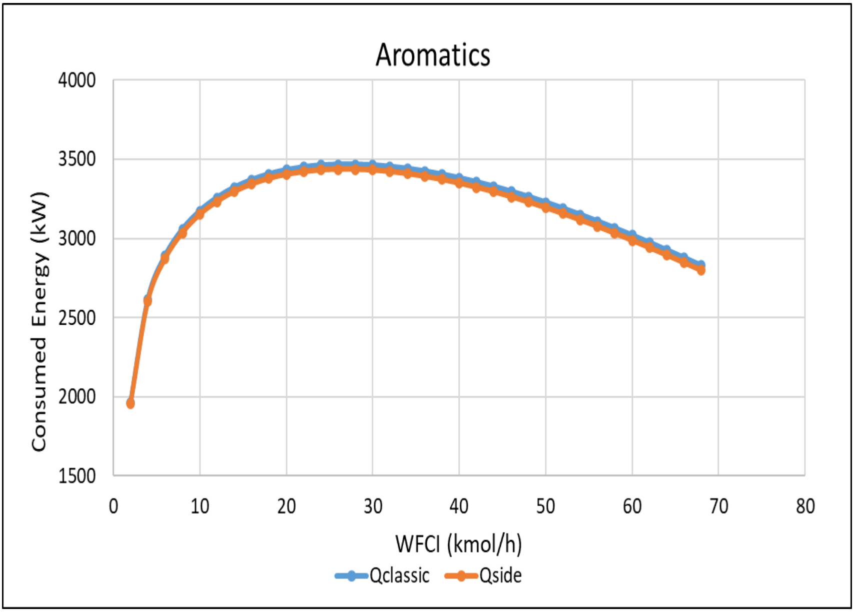

Figure 13: Energy consumed by side rectifier and conventional columns for a feed flow rate of 100 kmol/h

Although a lesser consumption of energy was seen for the mixture with higher content of the intermediate component but the overall savings by the side rectifier as compared to conventional columns is practically null, as only around 1.1% of overall can be observed in the figure 14 for higher amount of lighter component.

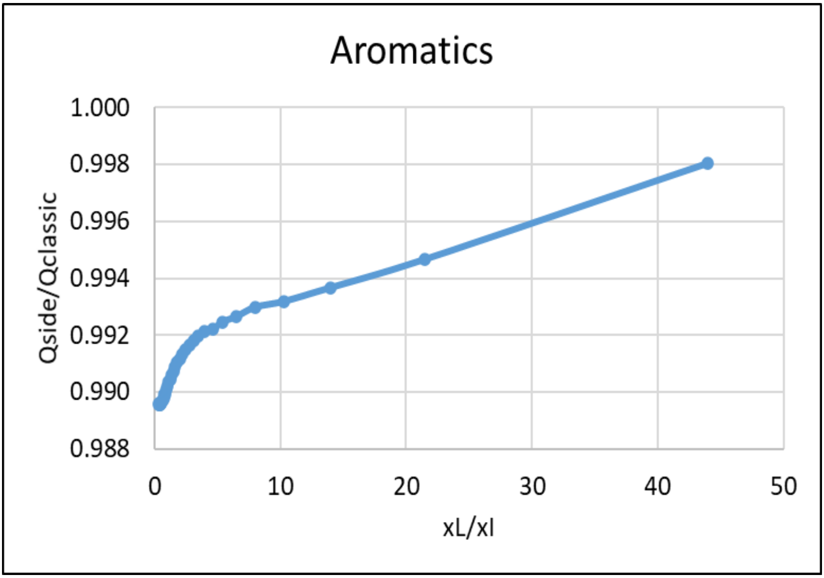

Figure 14: Energy comparison between side rectifier and conventional columns for a feed flow rate of 100 kmol/h

After observing a very low amount of energy savings obtained for the sensitivity analysis of the mixture for a fixed flow rate of heavy component, a further analysis was done by varying the respective flow rate and the simulation results are present in the Appendix3.

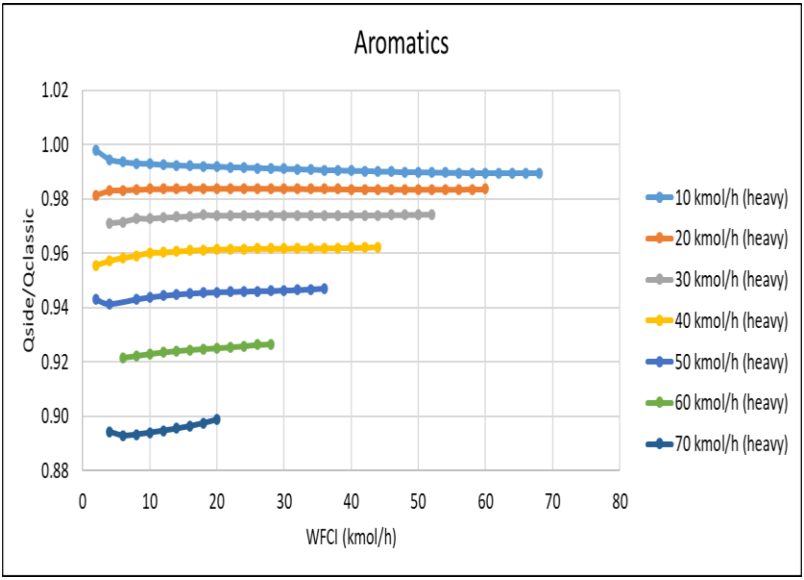

Figure 15: Energy comparison between side rectifier and conventional columns for different flow rates of heavy component.

A clear differences can be observed in the figure 14, as for a higher ratio of heavy component in the mixture a considerable amount of energy is saved by the side rectifiers with respect to the conventional columns, in case of flow rate of 70 kmol/h of heavy component in the feed around 11% of overall savings is observed.

From the results obtained it is quite clear that there is no situation in which the side columns provide great energy savings. The discrepancies in the literature may have come from the fact that the optimization of column is complicated because it has discrete variables and can present local minimums. For example, an increase in operating costs in terms of reflux and boiler energy, can be offset by a decrease in capital costs, like in the number of plates. Other variables such as the amount of heavy compound in the intermediate stream may have been left free, giving energy consumption that can be quite different.

6. CONCLUSIONS

After thoroughly analysing the results obtained from the simulation of two different types of configurations used for the separation, we can conclude that the energy savings obtained by using the side columns as an alternative for the conventional columns does not seems to have a big impact.

Another important aspect that was taken into account were the studies of different authors mentioned which shows an overall savings of around 26% and were focused on a fixed feed composition for certain components, while we have analysed all the different possibilities by performing a total of 22 rigorous simulations and still no significant savings are detected. The only case in which savings of around 11% was achieved was in the case of aromatics mixture in which the feed rate of heavy component was relatively high. But looking around the operational costs of both columns if the overall energy savings of the energetically integrated columns are lesser than 15% it does not pay off. This is literally because the installation of these types of columns generally requires more economic inversion rather than the conventional columns.

That is the main reason that despite being invented in the early 1970’s, the usage of these columns in the industry is still very limited because no one yet had established under which particular conditions side columns could provide significant energy savings.

FUTURE WORK

Although the use of side columns did not proportionate significant results in distillation of ternary ideal mixtures, but we cannot say that they will not be advantageous for other cases. For example, their capabilities can be tested while operating at different pressure while in our case the pressure was constant or can be tested in Extractive distillation as well.

Like as said before the research in these types of columns has been continuous since their introduction in the industry, a future work on situations proposed above can help find out whether the use of side columns can really be advantageous or not.

REFERENCES AND NOTES

1. Fang T., Ye Y., Xigang Y., Yiqing L., 2017. Influence of mixture and separation requirements on optimal configuration for ternary distillation. Huagong Xuebao/CIESC Journal, 68(2), 708-715.
2. Kumar S., Gupta S., Nanoti S.M, 2017. Techno-economic evaluation of top, middle, and bottom divided wall column configurations for benzene, toluene, and xylene processing in aromatic production plant, Separation Science and Technology, 52(1), 122-131.
3. Wang, L., Tian, F., Luo, Y., Yuan, X., Yu, G., 2018, A generalized ease of separation index for selection of optimal configuration of ternary distillation. Chemical Engineering Transactions, 69, pp. 241-246.
4. Tarjani, A.J., Toth, A.J., Nagy, T., (...), Fozer, D., Mizsey, P., 2018, Thermodynamic and Exergy Analysis of Energy-Integrated Distillation Technologies Focusing on Dividing-Wall Columns with Upper and Lower Partitions. Industrial and Engineering Chemistry Research, 57(10), pp. 3678-3684
5. Tututi-Avila, S., Medina-Herrera, N., Hahn, J., Jiménez-Gutiérrez, A., 2017, Design of an energy-efficient side-stream extractive distillation system. Computers and Chemical Engineering, 102, pp. 17-25.
6. Nicolae, M., 2017, Complex systems of distillation columns used in the production of the propylene oxide, Revista de Chimie, 68(1), pp. 28-34
7. Brito, K.D., Cordeiro, G.M., Figueirêdo, M.F., Vasconcelos, L.G.S., Brito, R.P., 2016, Economic evaluation of energy saving alternatives in extractive distillation process. Computers and Chemical Engineering, 93, pp. 185-196
8. Wang, E., Li, Z., Li, C., 2013, Simulation on application of dividing wall column in aniline distillation, Advanced Materials Research, 602-604, pp. 1299-1303
9. Wang, E., Huang, J., He, Y., Li, C., 2013, Study on simulation of nitrobenzene distillation using dividing wall column, Advanced Materials Research, 602-604, pp. 1364-1368
10. Tedder, D.W., Rudd, D.F., 1978, Parametric studies in industrial distillation: Part I. Design comparisons. AIChE Journal, 24(2), pp. 303-315
11. C. Triantafyllou, R. Smith, The design and optimization of fully thermally coupled distillation columns, Trans. Inst. Chem. Eng. 70 (1992) 118–132.
12. Hernández, S., 2008. Analysis of energy-efficient complex distillation options to purify bioethanol. Chem. Eng. Technol. 31 (4), 597–603.
13. Wu, Y.C., Hsu, P.H.-C., Chien, I.-L.L., 2013. Critical assessment of the energy-saving potential of an extractive dividing-Wall column. Ind. Eng. Chem. Res. 52 (15),5384–5399.
14. Van Duc Long, N., Lee, M., 2013. Optimal retrofit design of extractive distillation to energy efficient thermally coupled distillation scheme. AIChE J. 59 (4),1175–1182.
15. M. Xia, B. Yu, Q. Wang, H. Jiao, C. Xu. Design and control of extractive dividing-wall column for separating methylal-methanol mixture. Ind. Eng. Chem. Res., 51 (2012), pp. 16016-16033
16. Sun L, Wang Q, Li L, Zhai J, Liu Y. Design and control of extractive dividing wall column for separating benzene/cyclohexane mixtures. Ind Eng Chem Res 2014;53(19):8120e31.
17. Lu (Lu and Lü, 2005) showed that feed composition as well as ESI can have a tremendous influence on the selection of optimum distillation sequence in ternary mixtures:
18. Lu E X, Lü X H., 2005, Thermal coupling distillation and its selection principle[J]. Chemical Engineering (China), 33(2): 9-12.

ACRONYMS

xA	Molar fraction of Light component
xB	Molar fraction of Intermediate component
xC	Molar fraction of Heavy component.
Qside	Energy consumed by Side Rectifier
Qclassic	Energy consumed by Conventional columns connected in series
xL/xI	Ratio between Light and Intermediate component in the feed
η	Carnot efficiency of the column
FFR	Feed flow rate
HFR	Heavy component flow rate in the feed
WFCH	Flow rate of Heavy component in the feed
WFCI	Flow rate of Intermediate component in the feed
WFCL	Flow rate of Light component in the feed
vary1	Variable 1
vary2	Variable 2
vary3	Variable 3

APPENDICES

APPENDIX 1: RESULTS OF ALKANES MIXTURE

In this section the results of simulations of all different cases that were proposed for the mixture of alkanes are represented. Table 10 shows a series of 20 simulations for a ternary mixture of alkanes composed by **pentane, hexane and decane.** The overall feed flow rate is kept constant, i.e. 120 kmol/h, and the flow rate of heavy compound (decane -WFCH) is kept at 10 kmol/h. The flowrates of pentane (WFCL) and hexane (WFCI) vary to study the influence of the concentration of light compounds in an ideal mixture. The column Q corresponds to the energy consumed by the reboiler of an intensified scheme with a side rectifier. The increase of intermediate boiling compound in the mixture increase the energy requirements. When the lighter compound becomes under 1/3 of the mixture, then a rather flat energy consumption is obtained. The columns Q1 and Q2 correspond to the reboilers consumption of columns of a sharp classical process scheme. Q1 is the energy to separate the light compound from the rest and Q2 is the energy to separate the intermediate and heavy compounds. When a large amount of light compound is present, most of the energy is consumed in the first column where the light compound is recovered. When the molar ratio between light and intermediate compound (column xL/xI) becomes around 0.36 then the energy consumed by both columns is similar. For higher proportions of intermediate compound, the highest energy is consumed in the second column as expected. The sum of Q1 plus Q2 presented in the column Qclassic show that the overall energy consumed by the classic schemes is always higher than the energy consumed by the intensified scheme. The column Qside/Qclassic shows the ratio between the energy consumption of the intensified and the classical scheme. In any of the proportions of light and intermediate compounds the saving is between 1 to 2 %, therefore the energy savings does not justify the use of the intensified scheme.

Table 10. Simulation results for the mixture of Alkanes with feed rate of 100 kmol/h

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	10	4	86	890.09	85.91	818.87	21.50	904.77	890.09	0.9838
OK	10	6	84	967.01	113.87	868.49	14.00	982.36	967.01	0.9844
OK	10	8	82	1009.19	137.14	887.79	10.25	1024.93	1009.19	0.9846
OK	10	10	80	1037.46	158.18	895.24	8.00	1053.43	1037.46	0.9848
OK	10	22	68	1125.17	269.49	872.06	3.09	1141.55	1125.17	0.9857
OK	10	28	62	1152.73	321.96	847.15	2.21	1169.11	1152.73	0.9860
OK	10	52	38	1232.27	526.65	720.67	0.73	1247.32	1232.27	0.9879
OK	10	56	34	1241.89	560.37	696.28	0.61	1256.65	1241.89	0.9883
OK	10	66	24	1260.45	644.39	630.28	0.36	1274.67	1260.45	0.9888
OK	10	68	22	1262.85	661.16	616.00	0.32	1277.16	1262.85	0.9888
OK	10	70	20	1264.78	677.91	601.25	0.29	1279.15	1264.78	0.9888
OK	10	72	18	1267.45	694.67	585.91	0.25	1280.58	1267.45	0.9897
OK	10	74	16	1268.40	711.37	569.86	0.22	1281.23	1268.40	0.9900
OK	10	78	12	1267.03	744.79	534.43	0.15	1279.23	1267.03	0.9905
OK	10	80	10	1263.53	761.48	513.88	0.13	1275.36	1263.53	0.9907
OK	10	82	8	1256.40	778.16	489.66	0.10	1267.82	1256.40	0.9910

Table 11 Simulation results for the mixture of Alkanes with total feed rate of 120 kmol/h and fixed feed rate of 10 kmol/h of heavy component.

Status	vary 1 WFCH (kmol/h)	vary 2 WFCI (kmol/h)	vary 3 WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	10	12	98	1239.12	176.05	1079.71	8.17	1255.76	1239.12	0.9867
OK	10	18	92	1295.54	231.95	1080.76	5.11	1312.71	1295.54	0.9869
OK	10	22	88	1321.77	267.72	1071.74	4.00	1339.45	1321.77	0.9868
OK	10	28	82	1354.43	320.22	1051.78	2.93	1372.00	1354.43	0.9872
OK	10	44	66	1420.29	457.26	980.51	1.50	1437.77	1420.29	0.9878
OK	10	60	50	1470.05	592.35	894.78	0.83	1487.12	1470.05	0.9885
OK	10	68	42	1490.11	659.48	847.35	0.62	1506.83	1490.11	0.9889
OK	10	72	38	1500.13	692.97	822.38	0.53	1515.35	1500.13	0.9900
OK	10	76	34	1507.51	726.41	796.46	0.45	1522.88	1507.51	0.9899
OK	10	78	32	1510.80	743.12	783.11	0.41	1526.22	1510.80	0.9899
OK	10	80	30	1513.80	759.81	769.46	0.38	1529.27	1513.80	0.9899
OK	10	82	28	1516.47	776.49	755.49	0.34	1531.98	1516.47	0.9899
OK	10	84	26	1518.79	793.16	741.16	0.31	1534.32	1518.79	0.9899
OK	10	86	24	1520.69	809.83	726.41	0.28	1536.24	1520.69	0.9899
OK	10	90	20	1522.96	843.12	695.37	0.22	1538.49	1522.96	0.9899
OK	10	92	18	1523.07	859.75	678.82	0.20	1538.57	1523.07	0.9899
OK	10	94	16	1522.20	876.37	661.29	0.17	1537.66	1522.20	0.9899
OK	10	96	14	1519.98	893.03	642.40	0.15	1535.42	1519.98	0.9899
OK	10	98	12	1515.76	909.59	621.55	0.12	1531.15	1515.76	0.9900

Table 12 Simulation results for the mixture of Alkanes with total feed rate of 100 kmol/h and fixed feed rate of 20 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xI feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	20	4	76	944.29	114.90	856.20	19.00	971.10	944.29	0.9724
OK	20	8	72	1037.50	187.21	878.52	9.00	1065.73	1037.50	0.9735
OK	20	20	60	1128.25	326.45	829.78	3.00	1156.23	1128.25	0.9758
OK	20	22	58	1137.80	346.26	819.36	2.64	1165.62	1137.80	0.9761
OK	20	30	50	1170.95	422.01	775.44	1.67	1197.46	1170.95	0.9779
OK	20	32	48	1178.18	440.37	763.96	1.50	1204.33	1178.18	0.9783
OK	20	36	44	1191.39	476.61	740.44	1.22	1217.05	1191.39	0.9789
OK	20	38	42	1197.91	494.56	728.38	1.11	1222.94	1197.91	0.9795
OK	20	46	34	1219.97	565.42	677.97	0.74	1243.39	1219.97	0.9812
OK	20	56	24	1240.42	652.60	609.01	0.43	1261.61	1240.42	0.9832
OK	20	52	28	1233.29	617.88	637.53	0.54	1255.40	1233.29	0.9824

Table 13 Simulation results for the mixture of Alkanes with total feed rate of 100 kmol/h and fixed feed rate of 30 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xI feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	30	10	60	1074.09	257.72	856.47	6.00	1114.20	1074.09	0.9640
OK	30	12	58	1089.21	288.12	841.13	4.83	1129.25	1089.21	0.9645
OK	30	16	54	1113.27	341.62	811.15	3.38	1152.78	1113.27	0.9657
OK	30	18	52	1123.49	365.93	796.60	2.89	1162.53	1123.49	0.9664
OK	30	24	46	1149.40	433.01	754.05	1.92	1187.06	1149.40	0.9683
OK	30	28	42	1164.02	474.55	725.99	1.50	1200.55	1164.02	0.9696
OK	30	30	40	1170.69	494.69	711.92	1.33	1206.61	1170.69	0.9702
OK	30	34	36	1182.79	534.00	683.45	1.06	1217.45	1182.79	0.9715
OK	30	40	30	1198.24	591.16	639.71	0.75	1230.86	1198.24	0.9735
OK	30	52	18	1218.21	701.43	544.89	0.35	1246.32	1218.21	0.9774
OK	30	56	14	1220.41	737.36	509.42	0.25	1246.77	1220.41	0.9789
OK	30	58	12	1219.83	755.23	490.33	0.21	1245.56	1219.83	0.9793

Table 14 Simulation results for the mixture of Alkanes with total feed rate of 100 kmol/h and fixed feed rate of 40 kmol/h of heavy component.

Status	vary 1	vary 2	vary 3	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)							
OK	40	4	56	1006.15	150.16	904.23	14.00	1054.39	1006.15	0.9542
OK	40	10	50	1075.63	291.83	834.73	5.00	1126.56	1075.63	0.9548
OK	40	20	40	1125.96	442.87	731.22	2.00	1174.08	1125.96	0.9590
OK	40	22	38	1133.36	467.85	712.82	1.73	1180.68	1133.36	0.9599
OK	40	24	36	1140.19	491.85	694.80	1.50	1186.65	1140.19	0.9608
OK	40	26	34	1146.48	515.03	677.02	1.31	1192.05	1146.48	0.9618
OK	40	28	32	1152.28	537.53	659.38	1.14	1196.91	1152.28	0.9627
OK	40	30	30	1157.59	559.45	641.81	1.00	1201.27	1157.59	0.9636
OK	40	32	28	1162.43	580.89	624.23	0.88	1205.12	1162.43	0.9646
OK	40	42	18	1179.27	682.71	533.84	0.43	1216.55	1179.27	0.9694
OK	40	44	16	1180.95	702.28	514.77	0.36	1217.05	1180.95	0.9703
OK	40	50	10	1180.69	759.90	452.98	0.20	1212.89	1180.69	0.9735
OK	40	52	8	1177.44	778.81	429.35	0.15	1208.17	1177.44	0.9746
OK	40	54	6	1170.34	797.58	401.87	0.11	1199.45	1170.34	0.9757

Table 15 Simulation results for the mixture of Alkanes with total feed rate of 100 kmol/h and fixed feed rate of 50 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	50	2	48	954.23	83.43	916.03	24.00	999.46	954.23	0.9547
OK	50	6	44	1033.04	224.28	869.05	7.33	1093.33	1033.04	0.9449
OK	50	16	34	1089.68	429.54	718.38	2.13	1147.93	1089.68	0.9493
OK	50	18	32	1096.87	460.57	693.43	1.78	1154.00	1096.87	0.9505
OK	50	20	30	1103.29	489.76	669.45	1.50	1159.21	1103.29	0.9518
OK	50	24	26	1114.09	543.94	623.44	1.08	1167.38	1114.09	0.9544
OK	50	26	24	1118.54	569.37	601.05	0.92	1170.42	1118.54	0.9557
OK	50	28	22	1122.37	593.93	578.86	0.79	1172.80	1122.37	0.9570
OK	50	30	20	1125.58	617.75	556.75	0.67	1174.51	1125.58	0.9583
OK	50	32	18	1128.15	640.93	534.59	0.56	1175.53	1128.15	0.9597
OK	50	34	16	1130.05	663.56	512.25	0.47	1175.81	1130.05	0.9611
OK	50	36	14	1131.22	685.70	489.60	0.39	1175.29	1131.22	0.9625
OK	50	38	12	1131.52	707.42	466.43	0.32	1173.84	1131.52	0.9639
OK	50	40	10	1130.72	728.76	442.44	0.25	1171.20	1130.72	0.9654
OK	50	42	8	1128.29	749.76	417.03	0.19	1166.79	1128.29	0.9670

Table 16 Simulation results for the mixture of Alkanes with total feed rate of 100 kmol/h and fixed feed rate of 60 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCl (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	60	6	34	1003.93	240.44	832.70	5.67	1073.14	1003.93	0.9355
OK	60	8	32	1016.48	295.90	790.25	4.00	1086.15	1016.48	0.9359
OK	60	10	30	1026.39	344.70	750.79	3.00	1095.49	1026.39	0.9369
OK	60	14	26	1041.50	428.29	679.70	1.86	1107.99	1041.50	0.9400
OK	60	16	24	1047.30	465.00	647.11	1.50	1112.11	1047.30	0.9417
OK	60	18	22	1052.13	499.16	615.96	1.22	1115.12	1052.13	0.9435
OK	60	20	20	1056.10	531.26	585.86	1.00	1117.12	1056.10	0.9454
OK	60	22	18	1059.22	561.63	556.55	0.82	1118.18	1059.22	0.9473
OK	60	24	16	1061.53	590.55	527.76	0.67	1118.31	1061.53	0.9492
OK	60	28	12	1063.61	644.91	470.85	0.43	1115.76	1063.61	0.9533
OK	60	30	10	1063.20	670.67	442.19	0.33	1112.86	1063.20	0.9554
OK	60	32	8	1061.48	695.64	412.85	0.25	1108.50	1061.48	0.9576
OK	60	34	6	1057.53	719.95	381.70	0.18	1101.65	1057.53	0.9599

Table 17 Simulation results for the mixture of Alkanes with total feed rate of 100 kmol/h and fixed feed rate of 70 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	70	4	26	928.09	186.08	815.16	6.50	1001.24	928.09	0.9269
OK	70	6	24	940.56	254.96	762.07	4.00	1017.03	940.56	0.9248
OK	70	10	20	955.97	366.32	664.49	2.00	1030.82	955.97	0.9274
OK	70	12	18	960.78	413.53	619.95	1.50	1033.48	960.78	0.9297
OK	70	14	16	964.25	456.67	577.64	1.14	1034.31	964.25	0.9323
OK	70	16	14	966.52	496.49	537.15	0.88	1033.64	966.52	0.9351
OK	70	18	12	967.70	533.60	498.03	0.67	1031.63	967.70	0.9380
OK	70	20	10	967.84	568.43	459.92	0.50	1028.35	967.84	0.9412
OK	70	22	8	966.85	601.36	422.39	0.36	1023.75	966.85	0.9444
OK	70	24	6	964.32	632.67	384.64	0.25	1017.31	964.32	0.9479
OK	70	26	4	958.29	662.60	344.32	0.15	1006.92	958.29	0.9517

APPENDIX 2: RESULTS OF ALCOHOLS MIXTURE

In this section the results of simulations of all different cases that were proposed for the mixture of alcohols are represented.

Table 18 Simulation results for the mixture of Alcohols with feed rate of 100 kmol/h and fixed feed rate of 10 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
ok	10	2	88	1198.20	1171.70	40.61	44.00	1212.31	1198.20	0.9884
ok	10	4	86	1613.50	1548.80	78.70	21.50	1627.50	1613.50	0.9914
ok	10	6	84	1763.50	1669.90	108.80	14.00	1778.70	1763.50	0.9915
ok	10	10	80	1913.20	1763.70	161.73	8.00	1925.43	1913.20	0.9936
ok	10	20	70	2081.70	1815.80	282.32	3.50	2098.12	2081.70	0.9922
ok	10	30	60	2195.30	1813.00	398.39	2.00	2211.39	2195.30	0.9927
ok	10	40	50	2301.90	1804.20	512.93	1.25	2317.13	2301.90	0.9934

Table 19 Simulation results for the mixture of Alcohols with feed rate of 100 kmol/h and fixed feed rate of 20 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
ok	20	2	78	1,269.80	1,241.40	54.71	39.00	1,296.11	1,269.80	0.9797
ok	20	4	76	1,580.30	1,505.50	103.21	19.00	1,608.71	1,580.30	0.9823
ok	20	6	74	1,699.90	1,587.40	140.65	12.33	1,728.05	1,699.90	0.9837
ok	20	10	70	1,822.80	1,648.20	203.29	7.00	1,851.49	1,822.80	0.9845
ok	20	14	66	1,904.00	1,668.98	258.72	4.71	1,927.70	1,904.00	0.9877
ok	20	20	60	1,986.14	1,677.27	336.03	3.00	2,013.29	1,986.14	0.9865
ok	20	30	50	2,110.13	1,676.74	458.08	1.67	2,134.82	2,110.13	0.9884
ok	20	40	40	2,237.31	1,681.36	576.38	1.00	2,257.74	2,237.31	0.9910
ok	20	50	30	2,367.01	1,692.18	692.85	0.60	2,385.03	2,367.01	0.9924
ok	20	60	20	2,476.70	1,685.70	808.26	0.33	2,493.96	2,476.70	0.9931

Table 20 Simulation results for the mixture of Alcohols with feed rate of 100 kmol/h and fixed feed rate of 30 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
ok	30	2	68	1,293.47	1,265.31	65.57	34.00	1,330.88	1,293.47	0.9719
ok	30	4	66	1,520.81	1,440.30	121.83	16.50	1,562.13	1,520.81	0.9736
ok	30	6	64	1,623.03	1,492.56	164.91	10.67	1,657.47	1,623.03	0.9792
ok	30	10	60	1,722.40	1,528.02	236.11	6.00	1,764.12	1,722.40	0.9764
ok	30	16	54	1,826.55	1,540.20	326.00	3.38	1,866.20	1,826.55	0.9788
ok	30	20	50	1,885.24	1,542.48	381.39	2.50	1,923.87	1,885.24	0.9799
ok	30	30	40	2,028.10	1,551.89	510.29	1.33	2,062.18	2,028.10	0.9835
ok	30	40	30	2,174.69	1,571.13	633.00	0.75	2,204.13	2,174.69	0.9866
ok	30	50	20	2,303.70	1,578.30	752.62	0.40	2,330.92	2,303.70	0.9883

Table 21 Simulation results for the mixture of Alcohols with feed rate of 100 kmol/h and fixed feed rate of 40 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
ok	40	2	58	1273.52	74.56	1246.88	29.00	1321.44	1273.52	0.9637
ok	40	4	56	1437.16	137.57	1353.04	14.00	1490.60	1437.16	0.9641
ok	40	6	54	1514.05	185.21	1383.57	9.00	1568.78	1514.05	0.9651
ok	40	10	50	1611.11	263.72	1401.58	5.00	1665.30	1611.11	0.9675
ok	40	12	48	1649.51	298.29	1404.67	4.00	1702.96	1649.51	0.9686
ok	40	14	46	1685.18	330.90	1406.83	3.29	1737.73	1685.18	0.9698
ok	40	16	44	1719.47	362.01	1408.94	2.75	1770.95	1719.47	0.9709
ok	40	18	42	1753.14	391.96	1411.49	2.33	1803.45	1753.14	0.9721
ok	40	20	40	1786.58	420.99	1414.69	2.00	1835.68	1786.58	0.9733
ok	40	22	38	1820.04	449.25	1418.70	1.73	1867.95	1820.04	0.9744
ok	40	24	36	1853.61	476.91	1423.33	1.50	1900.24	1853.61	0.9755
ok	40	26	34	1887.23	504.04	1428.60	1.31	1932.64	1887.23	0.9765
ok	40	28	32	1920.79	530.74	1434.32	1.14	1965.07	1920.79	0.9775
ok	40	30	30	1954.10	557.07	1440.29	1.00	1997.36	1954.10	0.9783

Table 22 Simulation results for the mixture of Alcohols with feed rate of 100 kmol/h and fixed feed rate of 50 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
ok	50	6	44	1397.75	203.06	1261.43	7.33	1464.49	1397.75	0.9544
ok	50	8	42	1448.76	247.62	1267.84	5.25	1515.46	1448.76	0.9560
ok	50	10	40	1493.73	287.89	1271.76	4.00	1559.66	1493.73	0.9577
ok	50	12	38	1535.97	325.16	1275.51	3.17	1600.66	1535.97	0.9596
ok	50	14	36	1576.83	360.19	1279.99	2.57	1640.18	1576.83	0.9614
ok	50	16	34	1617.08	393.51	1285.48	2.13	1678.99	1617.08	0.9631
ok	50	18	32	1656.99	425.46	1291.95	1.78	1717.41	1656.99	0.9648
ok	50	20	30	1696.48	456.32	1299.16	1.50	1755.47	1696.48	0.9664
ok	50	22	28	1735.45	486.26	1306.77	1.27	1793.04	1735.45	0.9679
ok	50	24	26	1773.57	515.46	1314.49	1.08	1829.95	1773.57	0.9692
ok	50	26	24	1810.63	544.01	1321.88	0.92	1865.89	1810.63	0.9704
ok	50	28	22	1846.16	572.02	1328.37	0.79	1900.39	1846.16	0.9715
ok	50	30	20	1879.76	599.56	1333.52	0.67	1933.08	1879.76	0.9724
ok	50	32	18	1910.85	626.69	1336.58	0.56	1963.28	1910.85	0.9733
ok	50	34	16	1938.76	653.47	1337.22	0.47	1990.69	1938.76	0.9739
ok	50	36	14	1962.57	679.93	1333.98	0.39	2013.92	1962.57	0.9745

Table 23 Simulation results for the mixture of Alcohols with feed rate of 100 kmol/h and fixed feed rate of 60 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xI feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
ok	60	6	34	1272.05	219.22	1131.14	5.67	1350.36	1272.05	0.9420
ok	60	8	32	1327.54	266.72	1138.67	4.00	1405.39	1327.54	0.9446
ok	60	16	24	1524.62	421.94	1174.61	1.50	1596.54	1524.62	0.9549
ok	60	18	22	1569.58	455.77	1184.20	1.22	1639.97	1569.58	0.9571
ok	60	20	20	1612.32	488.39	1192.72	1.00	1681.11	1612.32	0.9591
ok	60	22	18	1652.37	519.93	1200.11	0.82	1720.03	1652.37	0.9607
ok	60	24	16	1689.11	550.61	1205.01	0.67	1755.62	1689.11	0.9621
ok	60	26	14	1721.87	580.56	1207.04	0.54	1787.60	1721.87	0.9632
ok	60	28	12	1749.45	609.87	1204.36	0.43	1814.23	1749.45	0.9643

Table 24 Simulation results for the mixture of Alcohols with feed rate of 100 kmol/h and fixed feed rate of 70 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xI feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
ok	70	12	18	1331.11	371.44	1044.92	1.50	1416.36	1331.11	0.9398
ok	70	14	16	1383.12	410.73	1055.80	1.14	1466.53	1383.12	0.9431
ok	70	16	14	1429.66	447.98	1063.80	0.88	1511.78	1429.66	0.9457
ok	70	18	12	1470.72	483.58	1067.76	0.67	1551.34	1470.72	0.9480
ok	70	20	10	1504.92	517.82	1066.03	0.50	1583.84	1504.92	0.9502

APPENDIX 3: RESULTS OF ACROMATICS MIXTURE

In this section the results of simulations of all different cases that were proposed for aromatic mixture are represented.

Table 25 Simulation results for the mixture of Aromatics with feed rate of 100 kmol/h and fixed feed rate of 10 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	10	2	88	1956.86	40.36	1920.33	44.00	1960.70	1956.86	0.9980
OK	10	4	86	2603.16	69.48	2547.64	21.50	2617.12	2603.16	0.9947
OK	10	6	84	2872.00	94.33	2795.96	14.00	2890.29	2872.00	0.9937
OK	10	8	82	3036.26	117.62	2939.48	10.25	3057.10	3036.26	0.9932
OK	10	10	80	3150.37	140.09	3032.53	8.00	3172.62	3150.37	0.9930
OK	10	12	78	3233.42	162.08	3095.26	6.50	3257.35	3233.42	0.9927
OK	10	14	76	3295.91	183.77	3137.15	5.43	3320.92	3295.91	0.9925
OK	10	16	74	3342.56	205.24	3163.54	4.63	3368.78	3342.56	0.9922
OK	10	18	72	3378.26	226.54	3178.55	4.00	3405.09	3378.26	0.9921
OK	10	20	70	3403.84	247.73	3183.70	3.50	3431.43	3403.84	0.9920
OK	10	22	68	3421.39	268.83	3180.86	3.09	3449.69	3421.39	0.9918
OK	10	24	66	3432.11	289.86	3171.20	2.75	3461.06	3432.11	0.9916
OK	10	26	64	3436.91	310.82	3155.61	2.46	3466.44	3436.91	0.9915
OK	10	28	62	3436.46	331.74	3134.78	2.21	3466.52	3436.46	0.9913
OK	10	30	60	3431.34	352.61	3109.27	2.00	3461.88	3431.34	0.9912
OK	10	32	58	3422.00	373.45	3079.52	1.81	3452.97	3422.00	0.9910
OK	10	34	56	3408.81	394.25	3045.97	1.65	3440.21	3408.81	0.9909
OK	10	36	54	3392.07	415.02	3008.80	1.50	3423.83	3392.07	0.9907
OK	10	38	52	3372.06	435.77	2968.33	1.37	3404.10	3372.06	0.9906
OK	10	40	50	3349.01	456.50	2924.78	1.25	3381.28	3349.01	0.9905
OK	10	42	48	3323.10	477.21	2878.16	1.14	3355.38	3323.10	0.9904
OK	10	44	46	3294.54	497.89	2829.24	1.05	3327.12	3294.54	0.9902
OK	10	46	44	3263.46	518.56	2777.58	0.96	3296.14	3263.46	0.9901
OK	10	48	42	3230.04	539.19	2723.74	0.88	3262.94	3230.04	0.9899
OK	10	50	40	3194.40	559.84	2667.14	0.80	3226.98	3194.40	0.9899
OK	10	52	38	3156.70	580.46	2608.75	0.73	3189.21	3156.70	0.9898
OK	10	54	36	3117.06	601.06	2548.37	0.67	3149.43	3117.06	0.9897
OK	10	56	34	3075.64	621.65	2486.13	0.61	3107.77	3075.64	0.9897
OK	10	58	32	3032.59	642.22	2422.16	0.55	3064.39	3032.59	0.9896
OK	10	60	30	2988.06	662.79	2356.74	0.50	3019.52	2988.06	0.9896
OK	10	62	28	2942.24	683.33	2289.97	0.45	2973.30	2942.24	0.9896
OK	10	64	26	2895.28	703.87	2221.93	0.41	2925.80	2895.28	0.9896
OK	10	66	24	2847.38	724.40	2152.98	0.36	2877.37	2847.38	0.9896
OK	10	68	22	2798.69	744.91	2083.21	0.32	2828.13	2798.69	0.9896

Table 26 Simulation results for the mixture of Aromatics with feed rate of 100 kmol/h and fixed feed rate of 20 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xI feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	20	2	78	1893.72	61.08	1868.89	39.00	1929.97	1893.72	0.9812
OK	20	4	76	2419.79	96.94	2364.57	19.00	2461.51	2419.79	0.9831
OK	20	6	74	2647.08	125.63	2566.49	12.33	2692.11	2647.08	0.9833
OK	20	8	72	2786.58	151.83	2681.43	9.00	2833.26	2786.58	0.9835
OK	20	10	70	2882.50	176.63	2753.63	7.00	2930.26	2882.50	0.9837
OK	20	12	68	2951.51	200.52	2799.52	5.67	3000.04	2951.51	0.9838
OK	20	14	66	3001.98	223.78	2827.30	4.71	3051.08	3001.98	0.9839
OK	20	16	64	3038.62	246.59	2841.56	4.00	3088.15	3038.62	0.9840
OK	20	18	62	3064.42	269.06	2845.25	3.44	3114.30	3064.42	0.9840
OK	20	20	60	3081.40	291.26	2840.21	3.00	3131.47	3081.40	0.9840
OK	20	22	58	3090.96	313.24	2827.96	2.64	3141.20	3090.96	0.9840
OK	20	24	56	3094.19	335.06	2809.47	2.33	3144.53	3094.19	0.9840
OK	20	26	54	3091.86	356.74	2785.50	2.08	3142.24	3091.86	0.9840
OK	20	28	52	3084.62	378.30	2756.68	1.86	3134.98	3084.62	0.9839
OK	20	30	50	3072.97	399.77	2723.50	1.67	3123.27	3072.97	0.9839
OK	20	32	48	3057.31	421.15	2686.36	1.50	3107.51	3057.31	0.9838
OK	20	34	46	3037.99	442.45	2645.58	1.35	3088.03	3037.99	0.9838
OK	20	36	44	3015.30	463.70	2601.34	1.22	3065.04	3015.30	0.9838
OK	20	38	42	2989.49	484.89	2554.07	1.11	3038.96	2989.49	0.9837
OK	20	40	40	2960.80	506.03	2503.92	1.00	3009.95	2960.80	0.9837
OK	20	42	38	2929.42	527.13	2451.03	0.90	2978.16	2929.42	0.9836
OK	20	44	36	2895.56	548.19	2395.56	0.82	2943.76	2895.56	0.9836
OK	20	46	34	2859.39	569.22	2337.84	0.74	2907.05	2859.39	0.9836
OK	20	48	32	2821.12	590.21	2278.11	0.67	2868.31	2821.12	0.9835
OK	20	50	30	2780.93	611.17	2216.31	0.60	2827.48	2780.93	0.9835
OK	20	52	28	2739.05	632.11	2152.74	0.54	2784.85	2739.05	0.9836
OK	20	54	26	2695.68	653.03	2087.69	0.48	2740.71	2695.68	0.9836
OK	20	56	24	2651.06	673.93	2021.33	0.43	2695.26	2651.06	0.9836
OK	20	58	22	2605.45	694.79	1953.94	0.38	2648.73	2605.45	0.9837
OK	20	60	20	2559.04	715.64	1885.74	0.33	2601.38	2559.04	0.9837

Table 27 Simulation results for the mixture of Aromatics with feed rate of 100 kmol/h and fixed feed rate of 30 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xI feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	30	4	66	2219.91	121.11	2164.93	16.50	2286.04	2219.91	0.9711
OK	30	6	64	2408.20	152.97	2325.60	10.67	2478.57	2408.20	0.9716
OK	30	8	62	2523.66	181.64	2412.71	7.75	2594.35	2523.66	0.9728
OK	30	10	60	2601.63	208.42	2465.92	6.00	2674.35	2601.63	0.9728
OK	30	12	58	2656.23	234.06	2495.35	4.83	2729.41	2656.23	0.9732
OK	30	14	56	2694.34	258.85	2508.99	4.00	2767.84	2694.34	0.9734
OK	30	16	54	2720.07	283.00	2510.56	3.38	2793.57	2720.07	0.9737
OK	30	18	52	2735.97	306.69	2501.73	2.89	2808.41	2735.97	0.9742
OK	30	20	50	2743.81	329.91	2487.33	2.50	2817.24	2743.81	0.9739
OK	30	22	48	2744.84	352.85	2465.21	2.18	2818.06	2744.84	0.9740
OK	30	24	46	2740.00	375.53	2437.40	1.92	2812.93	2740.00	0.9741
OK	30	26	44	2729.98	398.00	2404.56	1.69	2802.56	2729.98	0.9741
OK	30	28	42	2715.38	420.28	2367.25	1.50	2787.52	2715.38	0.9741
OK	30	30	40	2696.64	442.40	2325.86	1.33	2768.26	2696.64	0.9741
OK	30	32	38	2674.15	464.39	2280.79	1.19	2745.18	2674.15	0.9741
OK	30	34	36	2648.25	486.26	2232.37	1.06	2718.63	2648.25	0.9741
OK	30	36	34	2619.24	508.03	2180.88	0.94	2688.91	2619.24	0.9741
OK	30	38	32	2587.38	529.71	2126.56	0.84	2656.26	2587.38	0.9741
OK	30	40	30	2552.95	551.30	2069.71	0.75	2621.01	2552.95	0.9740
OK	30	42	28	2516.22	572.83	2010.33	0.67	2583.16	2516.22	0.9741
OK	30	44	26	2477.46	594.29	1949.04	0.59	2543.34	2477.46	0.9741
OK	30	46	24	2436.98	615.70	1885.97	0.52	2501.67	2436.98	0.9741
OK	30	48	22	2395.09	637.05	1821.51	0.46	2458.56	2395.09	0.9742
OK	30	50	20	2352.12	658.36	1755.87	0.40	2414.22	2352.12	0.9743
OK	30	52	18	2308.38	679.62	1689.47	0.35	2369.10	2308.38	0.9744

Table 28 Simulation results for the mixture of Aromatics with feed rate of 100 kmol/h and fixed feed rate of 40 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	40	2	58	1671.72	93.00	1656.61	29.00	1749.61	1671.72	0.9555
OK	40	4	56	2002.56	143.25	1948.73	14.00	2091.98	2002.56	0.9573
OK	40	6	54	2154.44	178.15	2069.91	9.00	2248.06	2154.44	0.9584
OK	40	8	52	2246.39	208.91	2133.09	6.50	2342.00	2246.39	0.9592
OK	40	10	50	2306.72	237.55	2164.61	5.00	2402.16	2306.72	0.9603
OK	40	12	48	2346.71	264.70	2178.80	4.00	2443.51	2346.71	0.9604
OK	40	14	46	2372.23	290.87	2178.20	3.29	2469.08	2372.23	0.9608
OK	40	16	44	2386.72	316.27	2167.13	2.75	2483.39	2386.72	0.9611
OK	40	18	42	2392.37	341.05	2147.57	2.33	2488.63	2392.37	0.9613
OK	40	20	40	2390.70	365.35	2121.10	2.00	2486.45	2390.70	0.9615
OK	40	22	38	2382.81	389.22	2088.69	1.73	2477.91	2382.81	0.9616
OK	40	24	36	2369.53	412.76	2051.11	1.50	2463.87	2369.53	0.9617
OK	40	26	34	2351.51	436.02	2008.95	1.31	2444.97	2351.51	0.9618
OK	40	28	32	2329.30	459.04	1962.63	1.14	2421.67	2329.30	0.9619
OK	40	30	30	2303.34	481.85	1912.88	1.00	2394.73	2303.34	0.9618
OK	40	32	28	2274.06	504.47	1859.75	0.88	2364.22	2274.06	0.9619
OK	40	34	26	2241.86	526.93	1803.74	0.76	2330.68	2241.86	0.9619
OK	40	36	24	2207.13	549.26	1745.20	0.67	2294.45	2207.13	0.9619
OK	40	38	22	2170.30	571.46	1684.55	0.58	2256.01	2170.30	0.9620
OK	40	40	20	2131.80	593.54	1622.24	0.50	2215.78	2131.80	0.9621
OK	40	42	18	2092.11	615.53	1558.71	0.43	2174.24	2092.11	0.9622
OK	40	44	16	2051.68	637.43	1494.44	0.36	2131.87	2051.68	0.9624

Table 29 Simulation results for the mixture of Aromatics with feed rate of 100 kmol/h and fixed feed rate of 50 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xI feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	50	2	48	1513.65	105.70	1499.34	24.00	1605.04	1513.65	0.9431
OK	50	4	46	1765.86	163.88	1712.02	11.50	1875.90	1765.86	0.9413
OK	50	8	42	1952.60	234.60	1835.91	5.25	2070.51	1952.60	0.9431
OK	50	10	40	1995.24	264.82	1849.19	4.00	2114.00	1995.24	0.9438
OK	50	12	38	2020.49	293.41	1845.97	3.17	2139.38	2020.49	0.9444
OK	50	14	36	2033.17	320.83	1830.89	2.57	2151.73	2033.17	0.9449
OK	50	16	34	2036.11	347.37	1806.65	2.13	2154.03	2036.11	0.9453
OK	50	18	32	2031.20	373.21	1775.01	1.78	2148.22	2031.20	0.9455
OK	50	20	30	2019.77	398.47	1737.20	1.50	2135.67	2019.77	0.9457
OK	50	22	28	2002.81	423.25	1694.14	1.27	2117.39	2002.81	0.9459
OK	50	24	26	1981.11	447.63	1646.54	1.08	2094.17	1981.11	0.9460
OK	50	26	24	1955.37	471.67	1595.04	0.92	2066.71	1955.37	0.9461
OK	50	28	22	1926.23	495.39	1540.26	0.79	2035.65	1926.23	0.9462
OK	50	30	20	1894.30	518.88	1482.75	0.67	2001.62	1894.30	0.9464
OK	50	32	18	1860.28	542.13	1423.14	0.56	1965.27	1860.28	0.9466
OK	50	34	16	1824.85	565.20	1362.13	0.47	1927.33	1824.85	0.9468
OK	50	36	14	1788.67	588.08	1300.43	0.39	1888.52	1788.67	0.9471

Table 30 Simulation results for the mixture of Aromatics with feed rate of 100 kmol/h and fixed feed rate of 60 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	60	6	34	1592.11	224.32	1503.48	5.67	1727.80	1592.11	0.9215
OK	60	8	32	1638.88	259.07	1518.07	4.00	1777.14	1638.88	0.9222
OK	60	10	30	1663.88	290.81	1511.99	3.00	1802.80	1663.88	0.9229
OK	60	12	28	1674.28	320.70	1492.16	2.33	1812.86	1674.28	0.9236
OK	60	14	26	1673.99	349.29	1462.26	1.86	1811.55	1673.99	0.9241
OK	60	16	24	1665.39	376.88	1424.57	1.50	1801.46	1665.39	0.9245
OK	60	18	22	1650.18	403.69	1380.65	1.22	1784.34	1650.18	0.9248
OK	60	20	20	1629.68	429.86	1331.70	1.00	1761.56	1629.68	0.9251
OK	60	22	18	1605.03	455.49	1278.76	0.82	1734.25	1605.03	0.9255
OK	60	24	16	1577.33	480.66	1222.91	0.67	1703.57	1577.33	0.9259
OK	60	26	14	1547.72	505.44	1165.24	0.54	1670.68	1547.72	0.9264
OK	60	28	12	1517.29	529.86	1107.63	0.43	1637.49	1517.29	0.9266

Table 31 Simulation results for the mixture of Aromatics with feed rate of 100 kmol/h and fixed feed rate of 70 kmol/h of heavy component.

	vary 1	vary 2	vary 3							
Status	WFCH (kmol/h)	WFCI (kmol/h)	WFCL (kmol/h)	Q (kW)	Q2(kW)	Q1(kW)	xL/xl feed	Qclassic (kW)	Qside (kW)	Qside/ Qclassic
OK	70	4	26	1221.47	201.45	1164.23	6.50	1365.68	1221.47	0.8944
OK	70	6	24	1275.79	245.82	1182.97	4.00	1428.79	1275.79	0.8929
OK	70	8	22	1300.80	282.55	1173.62	2.75	1456.17	1300.80	0.8933
OK	70	10	20	1308.65	315.78	1148.05	2.00	1463.83	1308.65	0.8940
OK	70	12	18	1305.00	346.91	1111.60	1.50	1458.51	1305.00	0.8948
OK	70	14	16	1293.25	376.58	1067.46	1.14	1444.04	1293.25	0.8956
OK	70	16	14	1275.93	405.16	1018.05	0.88	1423.21	1275.93	0.8965
OK	70	18	12	1255.24	432.88	965.49	0.67	1398.37	1255.24	0.8976
OK	70	20	10	1233.26	459.90	911.87	0.50	1371.76	1233.26	0.8990