

## Improving Conventional Distillation Configuration for Ternary Mixtures Separation

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Rigorous simulations at steady-state are conducted for the separation of two different ternary mixtures by conventional distillation with direct and indirect separation sequence. The studied chemical systems are (ethanol/n-propanol/n-butanol) and (benzene/toluene/m-xylene) with 99 mol % products purity at different feed compositions: (45/10/45), (33.3/33.3/33.3), and (10/80/10). In order to reduce the remixing effects in the first column a sidedraw stream is introduced at peak point composition of middle component as transfer stream to the second column. Economic optimization is carried out for the conventional and improved configurations based on energy consumption and total annual cost (TAC) as the objective function. The results indicate that improvements of thermodynamic performance of both columns are achievable and the maximum TAC saving is 29 % in case of indirect sequence and 19 % for direct sequence at low concentration of middle component.

### 1. Introduction

Distillation is one of the most energy intensive unit operations, reducing energy consumption and lowering operating and capital costs for distillation columns by finding modified configurations are still under investigation. However, for separation ideal ternary mixtures into pure product streams several configurations have been suggested. For example, Petlyuk column has been shown to provide the lowest energy demand and 30% energy saving compared with conventional direct and indirect sequences Halvorsen (1999). In spite of this feature, Petlyuk configuration has not gained a wide industrial application, to a certain extent because of the possible control problems that system might create with recycle streams. Salvador et al (2006) and Agrawal and Fidkowski (1998a) proposed alternative distillation schemes that show unidirectional flow, such configurations present better operational properties, thermodynamic efficiency equivalent to the Petlyuk column, and provide significant energy savings. Agrawal and Fidkowski (1998a) found that the modified direct and indirect sequence configurations together provide high thermodynamic efficiency for the wide range of feed compositions and relative volatilities than do the thermally coupled column configurations; however, they explained that due to their ability to either accept or reject heat at the intermediate temperatures of binary mixtures.

Hernandez and Jimenez (1999) have carried out a comparison between energy requirement and controllability properties for three complex columns including the Petlyuk column. They have found that the schemes with side columns are economically competitive with Petlyuk column only for mixtures of low intermediate composition and when B/C split is harder than A/B separation. Schemes with side columns show

better dynamic properties than Petlyuk column, and the amount of middle component has no effect on the control properties. In this work a modified configuration of conventional direct and indirect sequences are proposed to improve the thermodynamic efficiency of the conventional distillation.

## 2. Configurations studied

It is well known that high energy requirements are needed in conventional distillation sequences due to the remixing effects. For example, in the conventional direct sequence (Figure 1.a), the concentration of the intermediate component in the first column reaches a maximum below the feed stage and then decreases in the bottoms of the column, such an effect known as remixing, therefore more energy will be required in order to re-purify the binary mixture BC in the second column. A similar phenomenon is occurring in case of indirect sequence (Figure 1.b). To reduce or eliminate the remixing presented in direct sequence a liquid sidedraw stream is connected below the feed location at the stage of peak middle component concentration and transferred to the second column above the liquid feed stream (Figure 2.c). In case of indirect sequence a vapor sidedraw stream is connected above the feed stream at maximum concentration of middle component and transferred to the second column below the vapor feed stream (Figure 2.d).

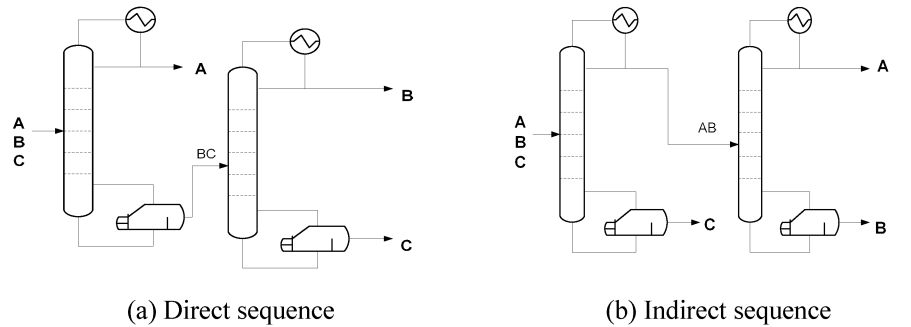


Figure 1: Conventional distillation sequences.

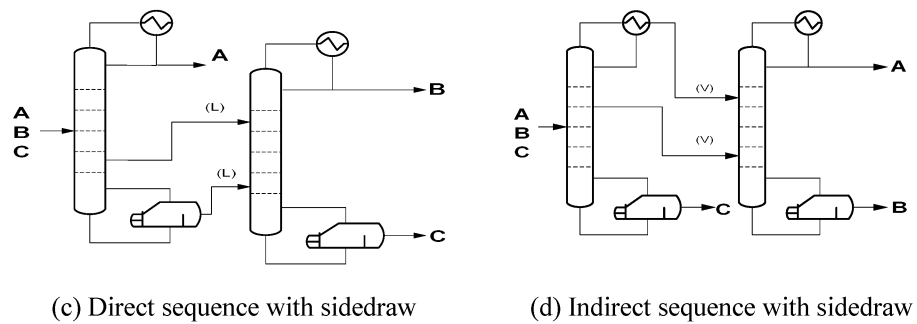


Figure 2: Improved conventional distillation sequences.

### 3. Rigorous case studies

Two different chemical systems are studied for the separation of ternary feed mixtures; alcohol system of (ethanol/n-propanol/n-butanol) and aromatic system of (benzene/toluene/m-xylene) for high product purity of 99 mol % of the three components are demanded. Throughout this work, A, B, and C will denote the light, intermediate, and heavy components respectively. The impurity in B product stream is equally distributed. The feed rate is 100 kgmol/hr and feed compositions are investigated for different values of feed compositions. Relative volatility and separation index (SI) of the case studies are given in Table 1.

HYSYS simulation package is used for rigorous steady-state modelling of the two case studies with the following assumptions: (a) NRTL thermodynamic model is selected for the alcohol system and Peng Robenson thermodynamic property set is used for the aromatics; (b) feed and products streams are assumed to be saturated liquids at atmospheric pressure, (c) pumping is not considered in cost calculations, (d) maximum internal flows are at 70-75 % of the flooding velocity, (d) exchange minimum approach temperature (EMAT) = 10 °C, and (e) LP-steam and cooling water are utilities for reboiler and condenser duties respectively.

*Table 1: Relative volatility and separation index for rigorous cases studies*

Feed mixture (A/B/C)	Feed composition (mol %)	Relative volatility ( $\alpha_{AB}/\alpha_{BC}/\alpha_{AC}$ )	SI ( $\alpha_{AB}/\alpha_{BC}$ )
ethanol/n-propanol/n-butanol	45/10/45	2.02/2.31/4.67	0.87
	33.3/33.3/33.3	2.07/2.29/4.72	0.90
	10/80/10	2.15/2.23/4.79	0.96
benzene/toluene/m-xylene	45/10/45	2.45/2.33/5.70	1.05
	33.3/33.3/33.3	2.42/2.30/5.57	1.05
	10/80/10	2.36/2.25/5.31	1.05

The economic objective function in this work is to minimize total annual cost (TAC) which is considered to be the sum of utility cost (steam and cooling water) and equipment cost (purchase and instillation). Detailed cost equations and utility cost data are extracted from Emtir et.al (2005).

### 4. Optimization procedure

All studied schemes are simulated rigorously by HYSYS process simulator and the results of simulation are collected in HYSYS spreadsheet and then exported to Microsoft Excel where the final cost calculations for optimization are executed. Detailed column and heat exchanger costs are calculated using the default column and heat exchanger sizing of HYSYS after rigorous simulation. The capital costs are executed in the Excel spreadsheet based on the cost correlations of Douglas (1988), capital costs are updated from mid-1968 to annual 2005 by Marshal and Swift index. For each distillation configuration, the pressure, number of trays, sidedraw flow rate and feed location are considered as the optimization variables; they are manipulated until the optimal design is achieved. In every simulation run, optimization variables are changed, specifications and optimality are checked. The process simulations are stopped when the global optimal system design is reached based on minimum TAC.

## 5. Results and Discussion

Improved direct and indirect sequences are compared with conventional configurations in terms of energy and total annual costs saving. The results shown in Table 2 indicate that direct sequence is improved by introducing the sidedraw stream up to 19 % TAC saving in case of low middle component concentration for both chemical systems and the percentage of saving has been reduced to 8 % in case of equimolar feed, where as the saving is only 3 % for higher concentration of middle component. The results shown in Table 3 are indicating higher savings for the case of improved indirect sequence with maximum TAC saving of 29 % at low concentration of middle component, which is similar to the savings in Petlyuk column at same feed composition with 28 % TAC saving (Emtir et al, 2005). Significant saving is also achieved for indirect sequence by introducing feed streams to the second column as liquid phase although the results are not showing here. Comparing the studied chemical systems, alcohol system reveals higher saving due to performing the difficult separation last, which will lead to higher utilization of energy provided in the first column.

Table 2: Optimized results of direct sequence

Chemical system	Feed composition (mol %)	Direct sequence (base case)		Improved direct sequence			
		Energy consumption (MW)	TAC ( $10^5$ \$/yr)	Energy consumption (MW)	TAC ( $10^5$ \$/yr)	Energy saving (%)	TAC saving (%)
ethanol/	45/10/45	1.82	5.38	1.45	4.38	21	19
n-propanol	33.3/33.3/33.3	2.23	6.52	2.02	5.98	10	8
/n-butanol	10/80/10	2.79	8.05	2.71	7.89	3	2
benzene/	45/10/45	1.41	4.24	1.10	3.42	22	19
toluene/	33.3/33.3/33.3	1.72	5.11	1.56	4.67	9	8
m-xylene	10/80/10	2.15	7.74	2.09	6.16	3	3

Table 3. Optimized results of indirect sequence

Chemical system	Feed composition (mol %)	indirect sequence (base case)		Improved indirect sequence			
		Energy consumption (MW)	TAC ( $10^5$ \$/yr)	Energy consumption (MW)	TAC ( $10^5$ \$/yr)	Energy saving (%)	TAC saving (%)
ethanol/	45/10/45	2.16	6.30	1.45	4.47	33	29
n-propanol	33.3/33.3/33.3	2.50	7.37	1.98	5.95	21	19
/n-butanol	10/80/10	2.87	8.26	2.65	7.80	8	6
benzene/	45/10/45	1.64	4.82	1.12	3.54	32	27
toluene/	33.3/33.3/33.3	1.90	5.62	1.55	4.78	18	15
m-xylene	10/80/10	2.22	6.52	2.05	6.07	8	7

Agrawal and Fidkowski (1998b) stated that it is more beneficial to have two interconnecting streams between the columns, one liquid and one vapor. This study has proved that introducing two liquid or vapor streams enhance the performance of direct and indirect conventional configurations. For example, in the improved indirect sequences, vapor stream which is withdrawn from partial condenser of the first column is fed to the second column, and other vapor feed stream withdrawn above the feed stage of the first column (Figure 2.d) provides thermodynamics benefits that significantly reduce the heat requirements for the second column. In case of improved

direct sequence, the liquid feed to the second column is the BC mixture withdrawn from the bottom of the first column, and sidedraw liquid feed is withdrawn below the feed stage of the first column at a point where the composition of component B reaches its peak value, the remixing effects are reduced in the first column leading to enhance the efficiency of the separation. The TAC saving calculated for the improved direct and indirect configurations (Tables 2-3) show better saving is obtained in the case of improved indirect sequences than the improved direct sequences. This result is in agreement with Agrawal and Fidkowski (1998a) who stated that the indirect split ( $IS_{LV}$ ) or side-stripper (SS) are more thermodynamic efficient than fully thermally coupled (Petlyuk column) and side-rectifier (SR) when the relative volatility between A and B is low. This is caused by the fact that, at the low value of  $\alpha_{AB}$  a relatively large vapor flow is needed to separate A from B, while the temperature of second column condenser ( $T_A$ ) is much closer to the bubble-point temperature of B ( $T_B$ ) than to the temperature of first column reboiler ( $T_C$ ). Thus its preferable to supply the large fraction of heat needed for the separation of A from B through a lower level heat source in the second column reboiler than to supply it at temperatures higher than  $T_B$ , where as in case of direct sequence it is not possible to supply heat at  $T_B$  which leads to greater degradation of some of the heat which is rejected in the first column condenser.

According to the heuristic rules presented by Glinos and Malone (1988), for the selection of the sequence for simple non-integrated distillation column, using direct sequence is favorable when  $X_A / (X_A + X_C) > (\alpha_{AB} - 1) / (\alpha_{AC} - 1)$ . But, withdrawing a sidedraw stream above the feed when the intermediate composition is 0.1 usually gives better saving compared to conventional direct and indirect configurations that is attributed to high recovery of B in the sidedraw, and as result of that the energy consumption in the second column will be significantly reduced. For the B-rich feed, it is found that the percentage of saving is quite low. This is due to the fact that the quantities of B are dominant and consequently the effect of remixing is not significant.

## 6. Conclusions

The improved direct and indirect configurations are found to have more energy saving compared to direct and indirect conventional configurations over the range of feed composition and relative volatilities examined so far. But the improved indirect sequences are better than the improved direct sequences when quantity of B in the feed is presented in smaller or equimolar amounts, due to the reduction of remixing effect and also providing a vapor sidedraw which enhance the thermodynamic performance of the configurations. Interestingly, it is found that at low concentration of middle component, the improved indirect is competitive to Petlyuk column with maximum TAC saving of 29 %. In contrast, at high concentration of middle component, the remixing was unavoidable, so that the TAC saving is inferior. The improved conventional configurations don't contain recycle streams, which might provide simple distillation systems to control and operate. The results are generally promising for the revamping of conventional distillation systems.

## 7. References

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