



SIMULATION ANALYSIS OF FULLY THERMALLY COUPLED DISTILLATION COLUMN

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ABSTRACT

Distillation is most important separation system which requires more energy to separation of multi-component system. Fully thermally coupled distillation system (FTCDS) requires less energy than other distillation system. In this study, three ternary mixtures are studied. FTCDS, conventional sequencing is simulated by using ASPEN PLUS with different parameters analysis. For those three mixtures, FTCDS and conventional sequencing methods energy consumption comparison studied.

Keywords: Fully thermally, Coupled distillation column, Design, Aspen plus.

INTRODUCTION

Distillation is one of the most important separation technologies. Distillation is most commonly used in chemical industries. It requires significant amount of energy. In all over world, 95% distillation is used for the separation. Whereas distillation itself consumes 3% of the world energy¹. Distillation can be used for binary or multi-component mixture; however the implementation of energy saving solution is often required. Different techniques are used for energy saving². The use of complex column like side stripper, side rectifier, thermally coupled columns reduces the overall heat duties. Divided wall distillation column (DWC) is also heat integrated system. In this configuration, use of heat exchangers are reduced.

Different configuration is used for multi-component separation. Numbers of conventional column are used. For this distillation, (n-1) columns, 2(n-1) condenser and reboiler are required for n-components separation³. Two methods are used for this configuration: (1) Direct sequencing and (2) indirect sequencing.

In direct sequencing method (Fig. 1a) for ternary component mixture first, of all the

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light component is separated in first column and heavy components are passed to the second column to separate. In indirect sequencing method (Fig. 1b) for ternary component mixture the heavy component is separated first and then light components are remixed with each other and that mixture is passed to the second column for separation⁴. For multi-component separation, fully thermally coupled columns are used. In that Petlyuk column and DWC are involved. Petlyuk column is invented in 1965 by Petlyuk and his coworkers. In this column, two columns are interconnected with each other, in which vapor and liquid are exchanged between two columns. For example, if ternary system ABC is separated into binary separation in first column AB in the top and BC in the bottom, AB fed to the top of the second column as a vapor and from same place liquid AB is given to first column which is prefractionator column as a reflux. Similarly, liquid BC is fed to the bottom of the second column and from same place vapor is given to the prefractionator column as boil-up. This connection eliminates the reboiler and condenser for the prefractionator column⁵, (Fig. 2). Pressure at the top part of the main column is lower than the top part of the prefractionator column and higher pressure at the bottom part of the main column than the prefractionator bottom part.

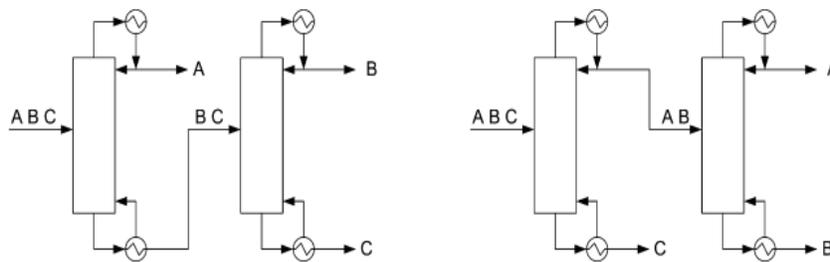


Fig. 1: Conventional column sequencing (a) direct sequencing (b) indirect sequencing

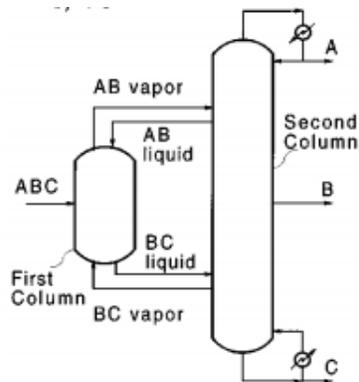


Fig. 2: Fully thermally coupled column-Petlyuk column

DWC was first invented by R. O. Wright⁶ for general purpose. DWCs first industrial application was used by BASF SE (1985). Up till 2010 it was recognized more than 100 DWC applications⁷. Distillation column with one vertical partition wall welded to the column wall, which is generally known as a dividing wall column (DWC), Fig. 3. In DWC nearly about 30% of energy savings are done compared to the direct and indirect sequencing columns. In DWC unnecessary mixing is avoided. The main advantage of DWC is to be used only one reboiler and one condenser. Proving it requires less capital cost and smaller footprints. Further applications and potentials are gained by recently introduced non welded technologies, which intensify more columns into one shell.

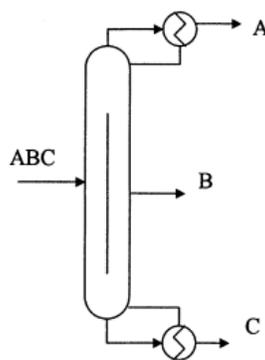


Fig. 3: DWC

Further applications and potentials are gained by recently introduced non welded technologies, which intensify more columns into one shell. DWC required less plot area so that shorter piping and electrical runs, a smaller storm runoff system, therefore heat loss is negligible. DWC is attractive not only for three component mixture also number of component mixture. DWC column is thermally equivalent to the Petlyuk column. Petlyuk column can be arranged in different column structure. In this structure composition, flow, temperature is same^{4,8}. For DWC, there is no separate model available in Aspen Plus. DWC is useful for separation in which production of detergents, aromatics, refining, hydro processing, reforming operation, etc. Comparatively DWC is more complex than conventional distillation column. For packed DWC Montz had patent in 1993 and for tray column in 2002.

Design procedure for DWC using ASPEN PLUS

Fully thermally coupled distillation, columns are designed by using simulation results. For that shortcut simulation method is used for the initial estimation for the rigorous simulation. In short cut design method, Fenske-Underwood-Gilliland equations are used. By

using Fenske equation minimum number of theoretical stages at total reflux was estimated; by using Underwood equation finite number of theoretical stages at minimum reflux. Feed stage is estimated by using Kirkbride equation⁹.

Shortcut distillation

Three shortcut columns are shown in the Fig. 4. Which is nearly equivalent to the fully thermally column distillation system (FTCDS). Shortcut column gives the necessary estimation for rigorous simulation. Column B1 is equivalent to prefractionator column in FTCDS and combination of column B2 and B3 are equivalent to main column. B2 bottom purity and B3 top purity should be same then can be added these two streams in to one and get flow for the side stream. In short cut distillation from first column vapor are passed to second column from the top of the first and liquid passes to the third column from the bottom of the first column. First column condenser is partial condenser and distillate is vapor stream. These are saturated vapor and saturated liquid¹⁰.

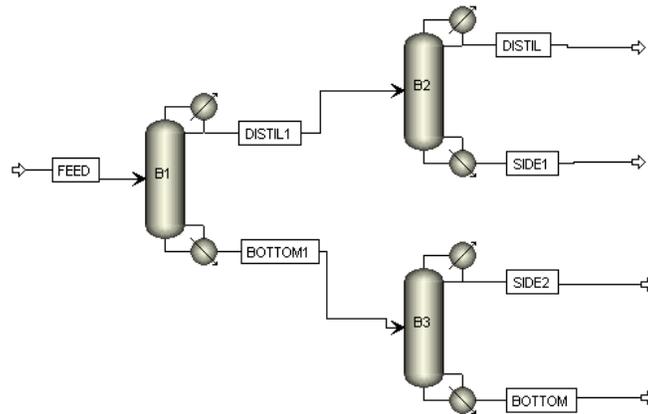


Fig. 4: Three shortcut column for simulation

DWC column is divided into 4 sections. Prefractionator section for feed mixture is equal to the first column (B1). Top section that is equal to the rectifying section of the second column (B2) and bottom section of the DWC is equal to stripping section of the third column (B3). Dividing wall section is the addition of the stripping section of the second column (B2) and rectifying section of the third column (B3). Side stream is the combination of the second and third column bottom and distillate, respectively¹¹.

DWC is equivalent to the Petlyuk column. In that prefractionator column is prefractionator side of DWC and main side is equal to the main column. Liquid and vapor recycle streams of Petlyuk column are liquid split and vapor split in the DWC, which are

located at top and bottom side of the dividing wall, respectively¹². Liquid split of the DWC is depends on the hydraulics of the column internals and vapor split depends on the location of the wall and pressure drop of the dividing section¹³.

Rigorous simulation

In ASPEN PLUS, DWC or Petlyuk configurations are not available in the unit operation libraries so that DWC is consider as the interconnecting of two columns with thermally coupling. For FTCDS simulation initial guesses were used, which given by shortcut distillation process.

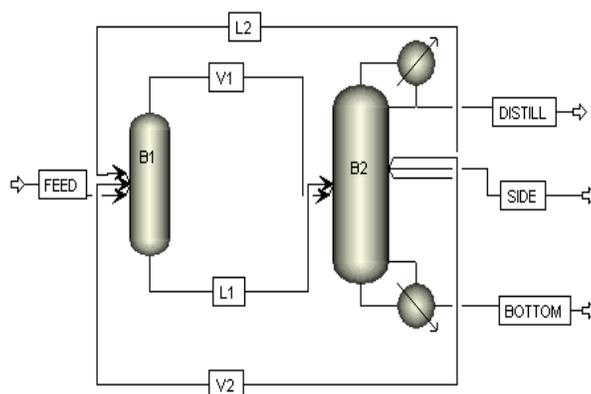


Fig. 5: Fully thermally coupled distillation system

First open the new simulation sheet and add the components, which involved in the process and choose thermodynamic model in base method. Then draw flow sheet for the FTCDS. In that first column is absorber (B1) from RadFrac model because that prefractionator column does not have reboiler and condenser. Then draw second column as distillation column (B2). Connect these two columns as shown in below Fig. 5. Give feed to B1 and vapor and liquid as a feed to B2 column. From main column recycle streams of vapor (V2) and liquid (L2) fed to the prefractionator column. Draw distillate, side stream, bottom stream lines from B2 column. Provide the data to this by shortcut estimation. Provide the number of stages to B1 and B2. Give stage location and flow rate to L2 and same stage location to V1. Give flow rate and stage location to V2 and same stage location to L1. B1 column do not have degree of freedom so that only number of stages, feed location and column pressure is given. B2 having more degree of freedom than B1. So that, for B2 column give feed stage location, recycle stream location and flow rate, distillate or bottom flow rate, side stream location and flow rate, column pressure same as B1¹⁴. After all parameters fill then simulate this sheet. By using trial and error achieve required purity and

minimum heat duties. Recycle stream that is liquid and vapor flows are more affected to the energy consumption in the FTCDS.

Case study

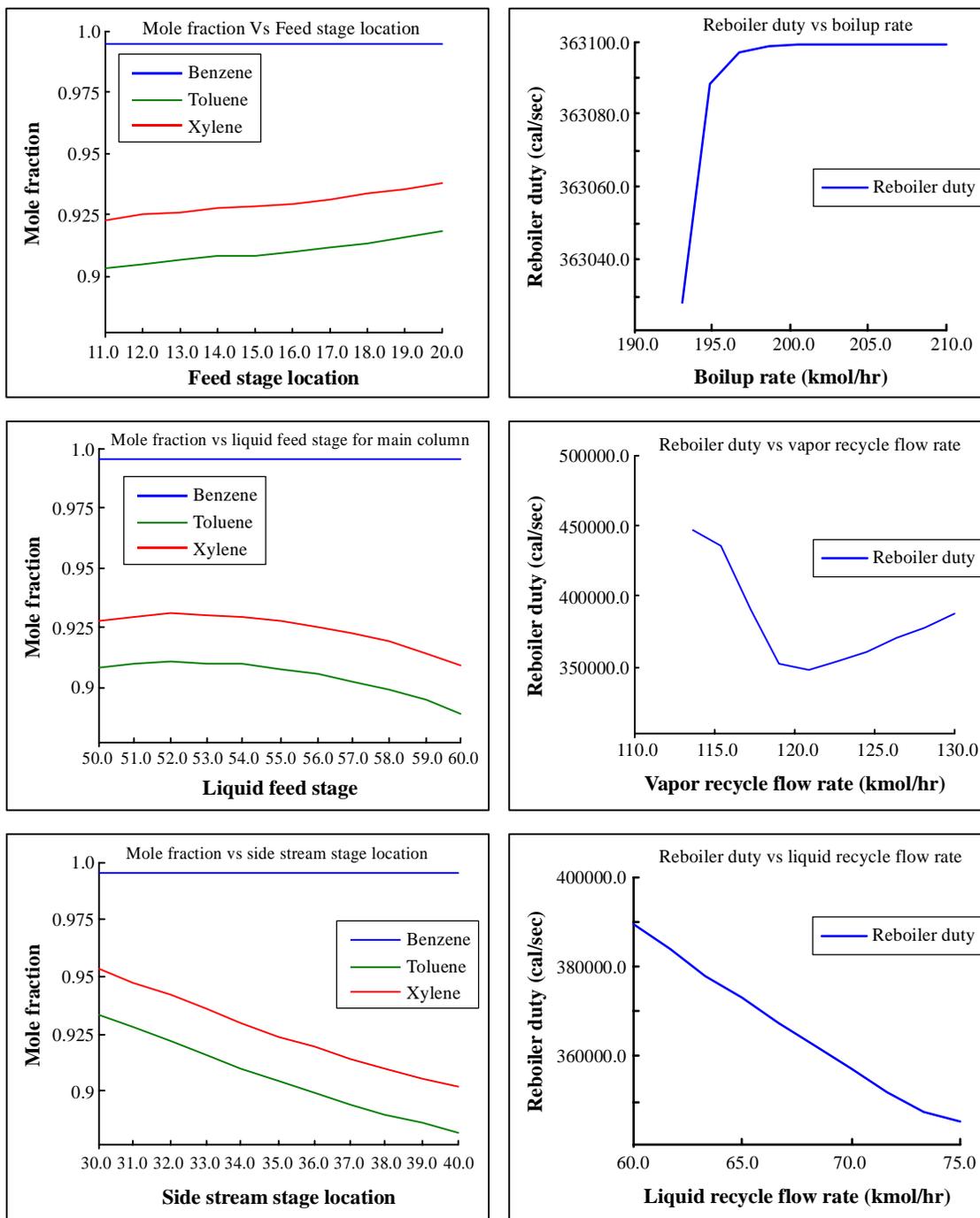
Three different ternary systems has been simulated and compared heat duty with conventional system. These three system conditions are given below:

Table 1: Specifications

Systems	1	2	3
	Benzene Toluene p-Xylene	Benzene Toluene Ethyl benzene	Ethanol 1-Propanol 1-Butanol
Feed compositions	0.33	0.33	0.1
	0.33	0.33	0.8
	0.34	0.34	0.1
Feed conditions	100 kmol/hr	100 kmol/hr	300 kmol/hr
	10 atm press	1.75 bar press	1 atm press
	Saturated liquid	Saturated liquid	Saturated liquid
Required mole %	99.5	99.5	99
	91	96	99
	92	96	99
Column pressure and model	10 atm	1.75 bar	1 atm
	Total condenser	Total condenser	Total condenser
	Peng-Rob	Peng-Rob	NRTL

RESULTS AND DISCUSSION

In this study, sensitivity analysis was used to analysis product purity and reboiler duty for FTCDS. Those graphs are shown in graph 1 below for system 1 (Benzene Toluene p-Xylene). Purity of side stream and bottom product linearly increases with feed stage location while a decrease with side stream location increases and distillate purity remains constant. When boil-up ratio increases then reboiler duty is also increases. Reboiler duty decreases with liquid recycle flow increases and with vapor recycle flow reboiler duty are decreases at some instant and then increases.



Graph 1: Sensitivity analysis graphs for purity of products and reboiler duty Vs different parameters

Table 2: shows the all optimum values for the FTCDS of three systems with energy saving compared to convention column sequencing. Above 35 % saving we got for these systems.

Table 2: Results for three systems

Systems	1	2	3
	Benzene toluene p-Xylene	Benzene toluene ethyl benzene	Ethanol 1-propanol 1-butanol
Number of stages for prefractionator column	34	36	34
Number of stages for main column	68	65	60
Feed stage for prefractionator column	16	18	14
Liquid feed stage for main column	18	17	14
Vapor feed stage for main column	53	53	51
Liquid flow rate from main column (Kmol/hr)	68	55	94.39
Vapor flow rate from main column (kmol/hr)	125	45	209.195
Side stream stage number	34	31	30
Side stream flow rate (kmol/hr)	33.5	32.65	241.145
Distillate rate (kmol/hr)	33	32.7943	29.0099
Reflux ratio	5.56081	4.7422	17.6141
Bottom rate (kmol/hr)	38.4977	34.5555	29.0099
Boilup rate (kmol/hr)	202.28	114	142.97
Boilup ratio	6.038	3.299	17.132
Condenser Duty (kw)	-1465.67	-1546.39	-6006.89
Reboiler Duty (kw)	1519.98	1090.61	5955.55
Saving compared with conventional sequencing in %	40.73	36.46	40.06

Conventional column sequencing

The simulation models for direct and indirect sequences were done in Aspen Plus. With the help of simulation which minimizes the sum of reboiler duties for two columns with desired purity constrains. For comparison with FTCDS minimum reboiler duty was selected. Table 3 shows system 1, Table 4 shows system 2, Table 5 shows system 3.

Table 3: Results for System 1

System	1			
Components	Benzene, toluene, p-xylene			
Conventional system	Direct sequence		Indirect sequence	
	B1	B2	B1	B2
Column	B1	B2	B1	B2
Number of stages	31	40	31	40
Feed stage	15	20	11	22
Distillate Rate (kmol/hr)	32.38	32.99	65.99	32.99
Reflux ratio	5.1	3.929	2.194	3.99
Bottom rate (kmol/hr)	67.62	34.63	33.99	32.99
Boilup rate (kmol/hr)	184.34	157.38	209.46	157.25
Boilup ratio	2.73	4.54	6.16	4.76
Condenser duty (Kw)	-1337.1176	-1173.67	-1538.48	-1119.00
Reboiler duty (kw)	1381.36	1183.18	1574.63	1134.27
Total reboiler duty (kw)	2564.54		2708.9	
Selected for comparison with FTCDS	2564.54			

Table 4: Results for System 2

System	2			
Components	Benzene, toluene, ethyl benzene			
Conventional system	Direct sequence		Indirect sequence	
	B1	B2	B1	B2
Column	B1	B2	B1	B2
Number of stages	51	35	51	35
Feed stage	22	18	19	27

Cont...

System		2		
Components		Benzene, toluene, ethyl benzene		
Conventional system	Direct sequence		Indirect sequence	
Distillate Rate (kmol/hr)	32.9	32.775	65.5	32.7
Reflux ratio	3.125	2.593	1.57	1.65
Bottom rate (kmol/hr)	67.1	34.325	34.5	32.8
Boilup rate (kmol/hr)	69.3809	111.58	106.54	81.016
Boilup ratio	1.034	3.251	3.088	2.47
Condenser duty (Kw)	-1114.50	-1057.88	-1489.82	-711.98
Reboiler duty (kw)	649.00	1067.51	1019.23	726.65
Total reboiler duty (kw)		1716.5		1745.88
Selected for comparison with FTCDS			1716.5	

Table 5: Results for System 3

System		3		
Components		Ethanol, 1-propanol, 1-butanol		
Conventional system	Direct sequence		Indirect sequence	
Column	B1	B2	B1	B2
Number of stages	52	32	52	32
Feed stage	14	20	26	16
Distillate Rate (kmol/hr)	29	241	269.85	27.95
Reflux ratio	10.41	1.301	1.2	10.25
Bottom rate (kmol/hr)	271	30	30.15	241.9
Boilup rate (kmol/hr)	302.61	536.25	558.17	290
Boilup ratio	1.12	17.88	18.51	1.19
Condenser duty (Kw)	-3577.77	-6407.32	-6670.05	-3400.01
Reboiler duty (kw)	3510.69	6425.97	6686.87	3337.63
Total reboiler duty (kw)		9936.66		10024.50
Selected for comparison with FTCDS			9936.66	

Analysis of the result

It can be observed that energy requirement for fully thermally coupled column is less than conventional column sequencing. Table 6 shows percent saving of FTCDS compared with conventional column sequencing.

Table 6: Energy saving

S. No.	System	Energy consumption		Energy % saving
		FTCDS	Conventional sequence	
1	Benzene, toluene, p-Xylene	1519.98	2564.54	40.73
2	Benzene, toluene, ethyl benzene	1090.61	1716.5	36.46
3	Ethanol, 1-propanol, 1-butanol	5955.55	9936.66	40.06

CONCLUSION

Distillation is a widely used separation technology. For distillation energy efficient configuration is required. DWC is more efficient than other methods. Different configurations were studied with rigorous simulation in Aspen Plus for three systems. Sensitivity analysis parameters are used to obtain values for producing results. According to results energy saving were obtained in fully thermally coupled column than conventional distillation column. It can be concluded that fully thermally coupled distillation column presents less reboiler duty.

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