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Modelling of Distillation Column that can Produce High Purity Aromatics from Catalytic Cracking or Reforming Unit using Aspen Hysys

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Abstract

The study involved modeling of a distillation column which can produce streams of high purity toluene and benzene from reformate of a catalytic cracking unit. Aspen Hysys was used to model and optimize a distillation column using Wilson as Fluid Package for physical properties of each component. For shot cut distillation column, employing available data yielded the lowest actual number of trays (31 trays). In the rigorous column (first distillation column), the following were obtained: optimal number of trays for the process (24), inlet feed stage (13 Ma), flow (top) rate (104 Kmol/hr), toluene in the bottom (0.0025 mole), e-benzene in distillate (0.009 mole), condenser duty (-6.157*10^6 KJ/h), reboiler duty (9.943*10^6 KJ/h), and external reflux ratio (0.806). In the second distillation column (short cut), optimum mole fraction of light key (n-heptane) in bottom (0.005 moles), optimum mole fraction of heavy key (toluene) in the distillate (0.005 moles), optimum number of trays (43) and reflux ratio (1.573), benzene flow rate (46Kmol/h), toluene (product) flow rate (25.76 or 26 Kmol/h), toluene purity (98.49%), condenser duty (-6432639.735), and reboiler duty (7285097.435). In the third Distillation Column (Short Cut), optimum mole fraction of light key (benzene) in bottom (0.020 moles), optimum mole fraction of heavy key (n-heptane) in the distillate (0.015 moles), optimum number of trays (37), reflux ratio (3.151), condenser duty (-5907570.031 KJ/hr), reboiler duty (6670143.257 KJ/hr), product rate (46.05 Kmol/hr), benzene purity (98.50%), and external reflux ratio (3.155). In this study, the distillation process was feasible and energy efficient. Therefore, Asphen Hysys can be used efficiently as a fast and easy tool to model and optimize a distillation column processes.

Keywords: Hysys, Distillation, Trays, Condenser, Reboiler duty.

Introduction

Distillation which originally involved a batch operation was the first method by which petroleum was refined **(Speight, 2007)**. Lower-value petroleum stocks are cracked in catalytic cracking unit to produce higher-value light and middle distillates. The process also produces light hydrocarbon gases, which are important feedstocks for petrochemicals. Fluid catalytic cracking (FCC) produces unsaturates, especially in the light hydrocarbon range C3–C5, which are used as petrochemical feedstocks and for alkylate production. In addition to hydrocarbon gases, FCC units produce gasolines with high octane numbers (due to the high aromatic content, branched paraffins and olefins), gas oils,

and tar. Benzene, toluene, and Xylene (BTX) and ethylbenzene are aromatic compounds that are normally present in large amount in the product of catalytic cracking unit and they can be separated employing distillation process (Gary and Handwerk, 2005; Kirk and Othmer, 1999-2012). The product from catalytic reformer (or cracking) contains C6 to C8 aromatics (benzene, toluene and ethylbenzene) together with other hydrocarbon components. Distillation is one of the method used by the petroleum and chemical industries either alone or in combination with other methods such as solvent extraction and crystallization to separate (or recover) these aromatics from hydrocarbon into its pure components which are used mainly by petrochemical industry with benzene having the greatest demand (Gary and Handwerk, 2001; Sami and Lewis, 2000).

Efficiency of distillation depends on a number of factors such as number of trays, reflux ratio, condenser duty, rebioler duty, and flow rate, and to obtain streams of BTX and e-thylbenzene products of high purity from catalytic cracking unit through distillation process, a well modeled and optimized distillation column is required. Most columns are designed to operate between 1.2 to 1.5 times minimum reflux ratio (Tham, 1997). The weaknesses of distillation process in separating aromatics are that number of columns and trays involved, energy requirement in terms of heating rate and cooling rate, and its capital cost as well as operating cost are all high. Extractive distillation or solvent extraction is good for separation of mixtures such as aromatics with close boiling point. However, the selectivity of the solvent, the boiling point of solvent and toxicity and the environmental impact are factors that make extractive distillation difficult and problematic (Lek-Utaiwan *et al*, 2010).

Aspen Hysys is one of the efficient tools which can model and optimize a distillation column. It is a tool for conceptual design, optimization, and performance monitoring for oil and gas production, gas processing, petroleum refining, and air separation industries. It offers comprehensive thermodynamics foundation for correct calculation of physical properties, transport properties, and phase behavior for the oil, gas and refining industries (Asphen Tech Inc, 2012). Hence, Hysys can be used to model distillation column used in petroleum industry for separation of crude oil into its component fractions and recovery of important chemical components or aromatics such as benzene from the refinery products. To demonstrate the Strength and weaknesses of distillation process when separating aromatics, some of the data and information obtained in the Hysys file are viewed. Therefore, the objective of this work was to obtain streams of high purity toluene and benzene (as close to 99 mol% as possible) from reformate of a catalytic cracking unit.

Materials and Methods

Methods and Process Roots

Aspen Hysys was used as the modeling tool and Wilson Fluid Package was selected for the component physical properties (Aspentech, 2014). Table 1 presents the physical properties of each component using Wilson Fluid Package. Tray type conventional distillation in two phases was used in this study and two process roots (Root A and Root B were considered in order to select a root that can achieve separation at high efficiency and low cost. Table 2 shows the distillation column particulars.

Table 1: Physical Properties of Each Component using Wilson as Fluid Package

Components	Molar Flow, Kmol/hr	Molar Fraction	Boiling Point
Toluene	26.000	0.130	110.649
Benzene	46.000	0.230	80.089
Ethyl benzene	6.000	0.030	136.200
Metha-xylene	24.000	0.120	139.115
1,3,5-trimethylbenzene	66.000	0.330	164.744
n-heptane	32.000	0.160	98.429
Total	200.000	1.000	

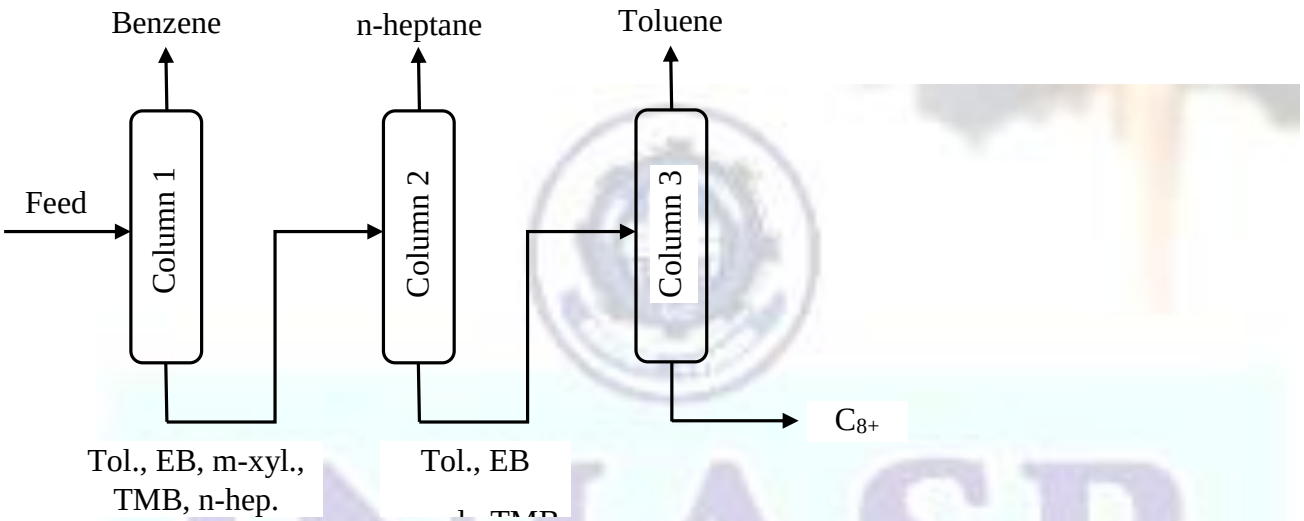
Table 2: Distillation Column Particulars

Feed Pressure	2 bar
Feed Temperature	50 °C
Condenser Pressure	1 bar
Reboiler Pressure	2 bar

External Reflux Ratio	1.2 x minimum reflux ratio

Process Roots Considered

In Root A (Figure I), Benzene was separated through the top from Toluene and other components in the first column (rigorous distillation column). N-heptane was separated from toluene, ethylbenzene and other components through the top in the second column. Then, toluene was separated from other C_8 mixtures through the top in the third column as shown in Figure I.



Tol (Toluene), EB (Ethylbenzene), m-xyl (m-xylene or meta-xylene), TMB (trimethylbenzene or tetramethylbenzene), C_{8+} (hydrocarbons with number of carbon atom from 8 and above

Figure I: Basic Block Diagram for Root A

In Root B (Figure 2), Toluene and the lighter were separated through the top from ethyl benzene and heavier components in the first column (rigorous distillation column). N-heptanes and benzene were separated from toluene through the top in the second column. Then, benzene was separated from n-heptanes through the top in the third column as shown in Figure 2.

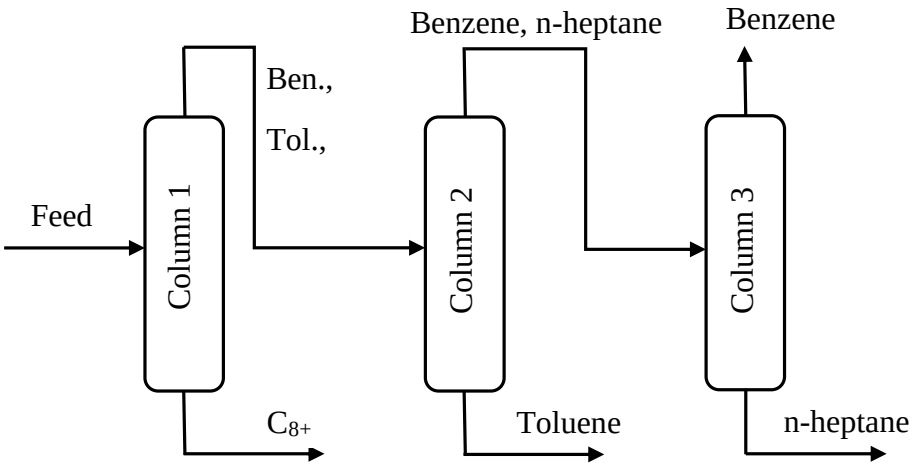


Figure 2: Basic Block Diagram for Root B

Initial or Preliminary Distillation (Short Cut Distillation Column)

Aspentech (2012) method as employed by Asteria *et al.* 2013) was used to model the short cut distillation column. Things considered and data used in designing initial short cut distillation column for root B were total flow rate of the three components: benzene, n-heptanes and toluene (104Kmol/hr), mole fraction of toluene as light key in bottom (0.0025) and mole fraction of e-benzene as heavy key in the distillate (0.0009). These yielded the required lowest actual number of trays, total flow rate of the products (benzene, n-heptanes and toluene), and external reflux ratio.

Rigorous Distillation Colum (Column 1

Datas from the short cut column were used to design the first column. In the rigorous column, number of trays and inlet feed stage were manipulated to get the optimum number of trays and inlet feed stage.

Short cut Distillation Column (Column 2)

In second column, the mole fraction of n-heptanes as the light key that will be in the bottom and mole fraction of toluene as the heavy key that will be in the distillate were monitored. In order to get the desired purity close to 99% of toluene at the desired amount of 26 Kmol per hour of flow rate, 0.005 mole of n-heptanes and 0.005 moles of toluene were chosen as optimum mole fraction of light key in bottom and heavy key in the distillate.

Short Cut Distillation Column (Column 3)

Aspentech (2012) method as employed by Asteria *et al.* 2013) was also used to model the second short cut distillation column. The mole fraction of benzene as the light key that will be in the bottom and mole fraction of n-heptanes as the heavy key that will be in the distillate were monitored. In order to get the desired purity close to 99% of benzene as distillate at the desired amount of 46 Kmol per hour of flow rate, 0.02 moles of benzene and 0.015 moles of n-heptanes were chosen as optimum mole fraction of light key in the bottom and heavy key in the distillate.

Results and Discussion

Table 3: Summary of data obtained in the Two Methods (Roots A and Root B)

	Method A	Method B
Number of Trays	169.00	123.00
Heater & Reboiler duty, KJ/hr	33,934,607.78	24,935,057.21
Pump Energy, KJ/hr	8,1796.80	9,525.40
Cooler & Condenser duty, KJ/hr	-29,820,984.43	-20,604,057.61
Benzene purity, %	98.09	98.50

Toluene purity, %	97.67	98.95

From Table 3, it can be seen that the total number of required trays for root A was 169 trays and total reboiler and heater energy requirement was 33,934,607.78KJ/hr, while 104 trays with total reboiler and heater energy of 24,935,057.21KJ/hr was required for root B. Therefore, method B (root B) was chosen for modeling of the distillation column in this study considering that root B was more economical in terms of energy requirement and cost of materials (trays) and it is more efficient (easier to get benzene and toluene of purity very close to 99% in root B than in root A). Therefore, Root B was discussed in detail in this study.

Short Cut Distillation Column

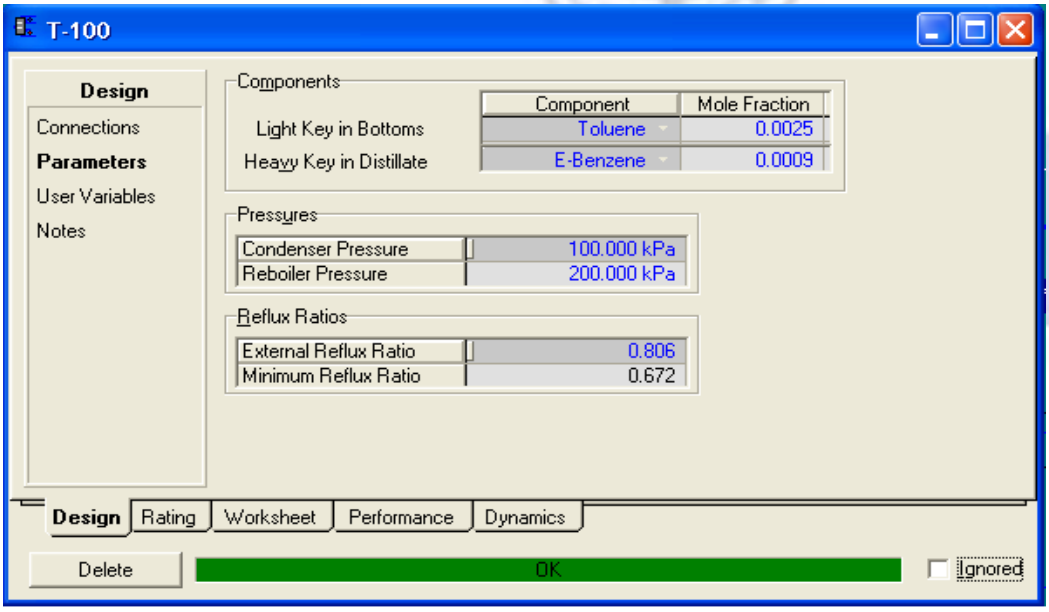


Figure 3: Optimum Parameters for Initial Short Cut Column

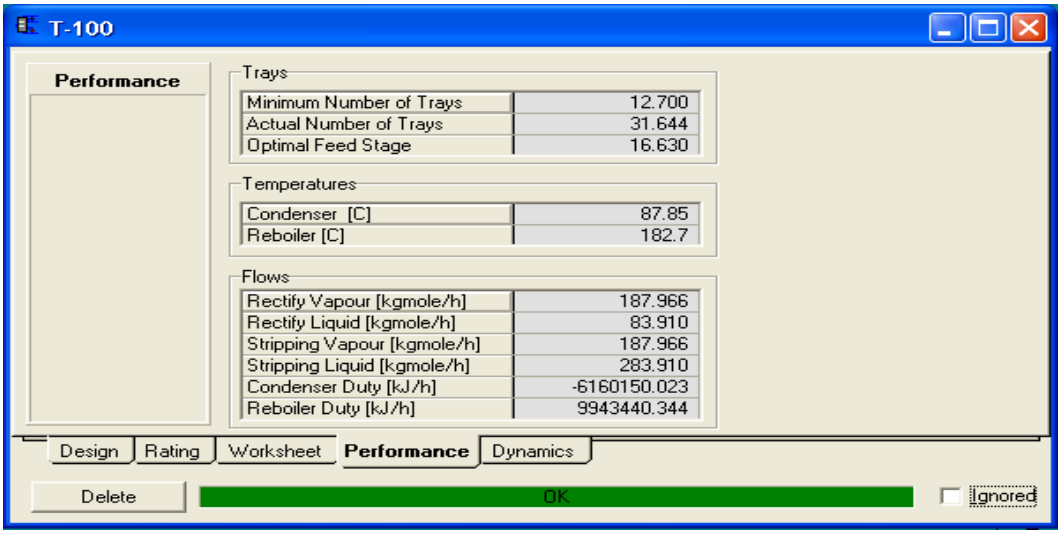


Figure 4: Optimum Performance for the Initial Short Cut Distillation Column

Table 4: data from initial Short Cut column

Toluene in Bottom, moles	E-benzene in Distillate, mole	Actual No of Trays	Condenser duty, KJ/hr	Reboiler Duty, KJ/hr	Product Rate Kmol/hr	Ext. Reflux ratio
0.01	0.0100	19.0000	-5400871.1400	9134402.8230		0.5090
0.0025	0.0090	31.0000	-6160150.0230	9943440.3440	104.1000	0.8060
0.0001	0.0001	50.0000	-6228860.3650	10016303.9530	104.0000	0.8290

Rigorous Distillation Colum (First Column or Column I)

The optimum number of trays and inlet feed stage of 24 and 13 Ma respectively and a corresponding flow rate of 104 for the bottom products were obtained using data from the initial short column. Using 23 trays in the rigorous column (first column) increased the number of trays needed in the second column. Therefore, optimal number of trays in the rigorous column for the process was 24.

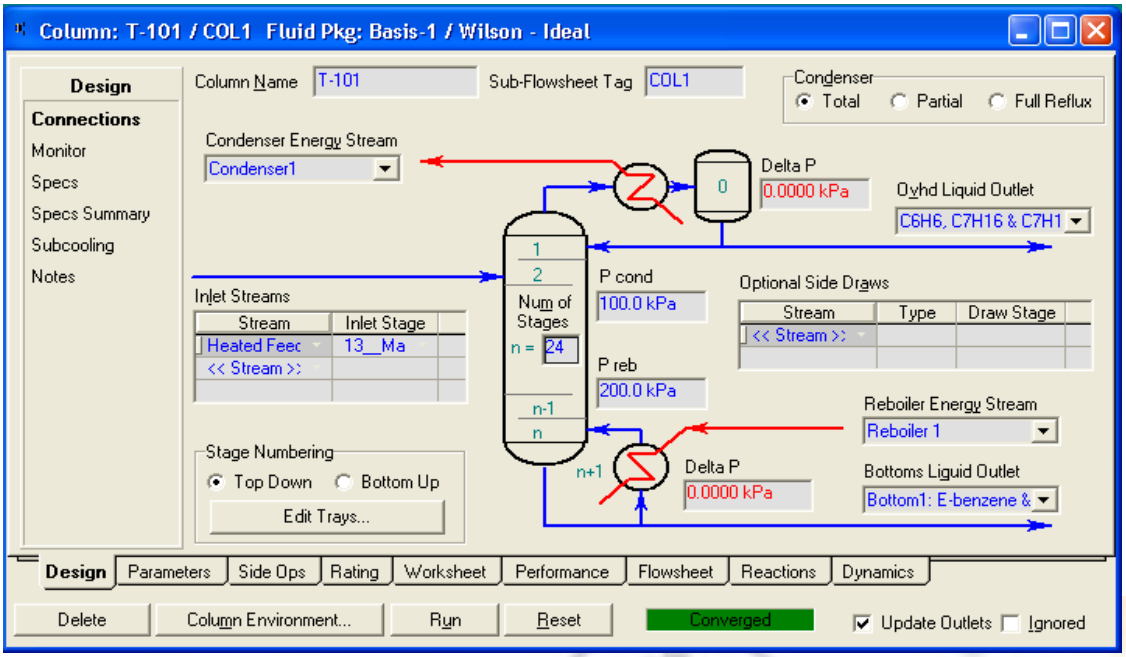


Figure 5: Column Design for the Rigorous Distillation Column Using Wilson Fluid Package

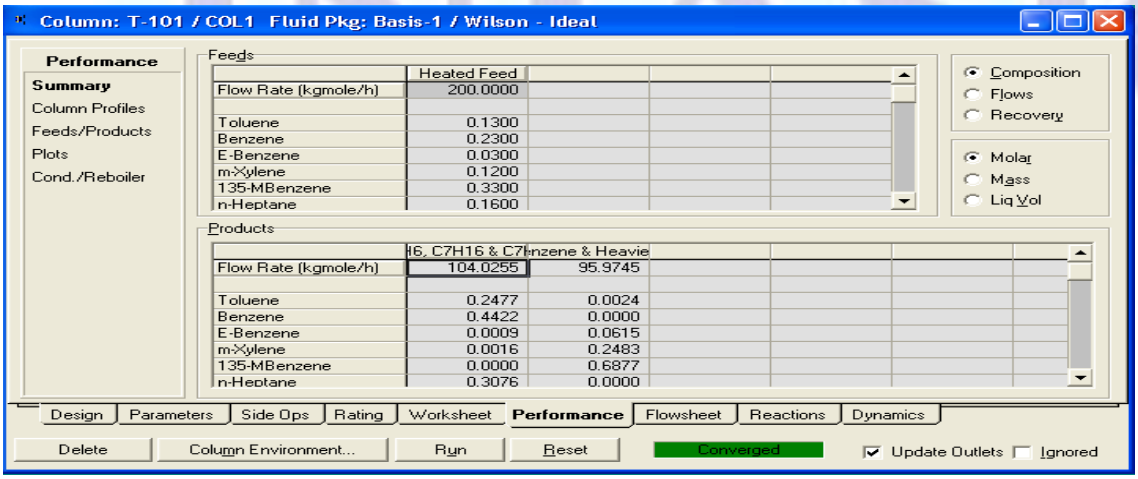


Figure 6: Performance of the Rigorous Distillation Column

Table 5: Data from First Column (Rigorous)

Toluene in Bottom, Moles	E-benzene in Distillate, Mole	Number of Trays	Condenser Duty	Reboiler Duty, KJ/h	Top Rate Kmol/h	Ext Reflux Ratio	Feed Inlet Stage
0.0025	0.009	31	6.168*10^6	9.953*10^6	104.2	0.806	15
0.0025	0.009	24	-6.157*10^6	9.943*10^6	104.	0.806	13
0.0025	0.009	23	-6.155*10^6	9.938*10^6	104	0.806	12
0.0025	0.009	20	-6.116*10^6	9.896*10^6	103.4	0.806	10

Short Cut Distillation Column (Second Column or Column 2)

In this column, Optimum number of trays (43) and reflux ratio (1.573) were obtained. Though, setting n-heptane as the light key in the bottom to 0.0100 and toluene as heavy key in the distillate to 0.0100 gave 37 trays and toluene purity of 97.98, it was not the optimum setting because this setting affected the performance of the third column and made it difficult to achieve desired purity (close to 99%) and flow rate (46 Kmol/h) of benzene with reasonable number of trays. Also, the 0.0005 and 0.0005 combinations for the light key and heavy key in bottom and distillate respectively gave toluene of flow rate equal to 26 Kmol/h and purity of 98.95%, but the number of trays required was much higher, therefore it did not give optimum design.

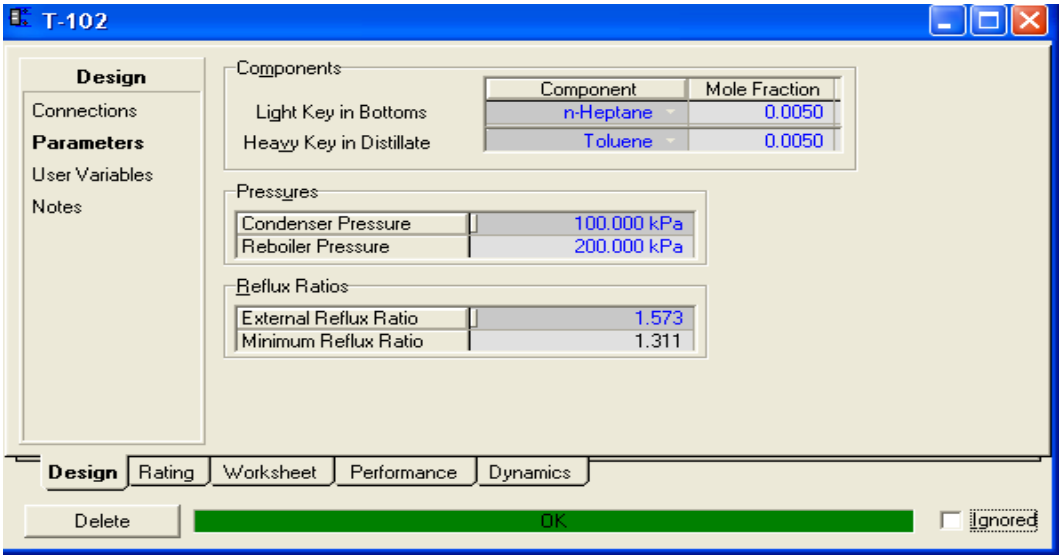


Figure 7: Optimum Parameters for second column (Short cut)

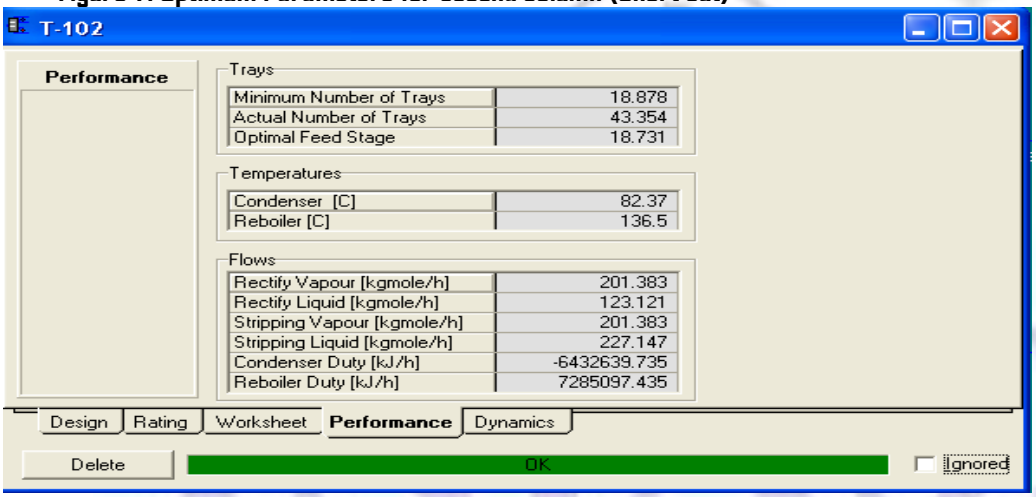


Figure 8: The optimum performance of the second column (Short cut)

Table 7: Data from Second Column (Toluene as product)

n-heptanes in Bottom, moles	Toluene in Distillate, mole	Actual No of Trays	Condenser duty (KJ/h)	Reboiler duty (KJ/h)	Product Rate Kmol/hr	Toluene Purity, %	Ext Reflux Ratio
0.0100	0.0100	37.0000	-6316533.2720	7167465.5910	25.5000	97.9800	1.5170
0.0050	0.0050	43.0000	-6432639.7350	7285097.4350	25.7600	98.4900	1.5730
0.0005	0.0005	63.0000	-644646.1580	7398435.3680	26.0000	98.9500	1.6270
0.0001	0.0001	87.0000	-652030.3540	7374441.8820	25.9900	98.9549	1.6190

Short Cut Distillation Column (Third Column or Column 3)

In this column, optimum number of trays (37) and external reflux ratio (3.155) were obtained with condenser duty (-5907570.031 KJ/hr), reboiler duty (6670143.257 KJ/hr), product (benzene) flow rate (46.05 Kmol/hr), and benzene purity (98.5%) which was close to the desired purity (99%) and flow rate of (46 Kmol/hr).

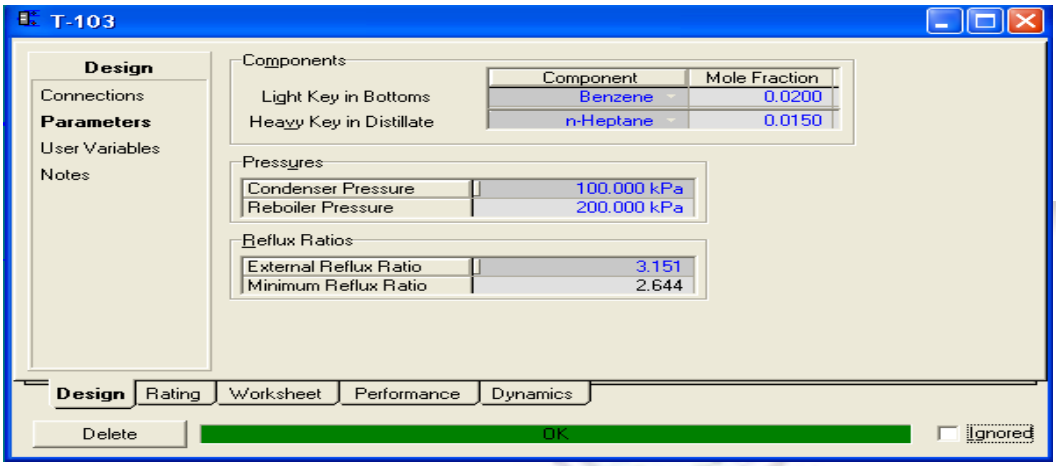


Figure 9: Optimum Parameters for Third Column (Short Cut)

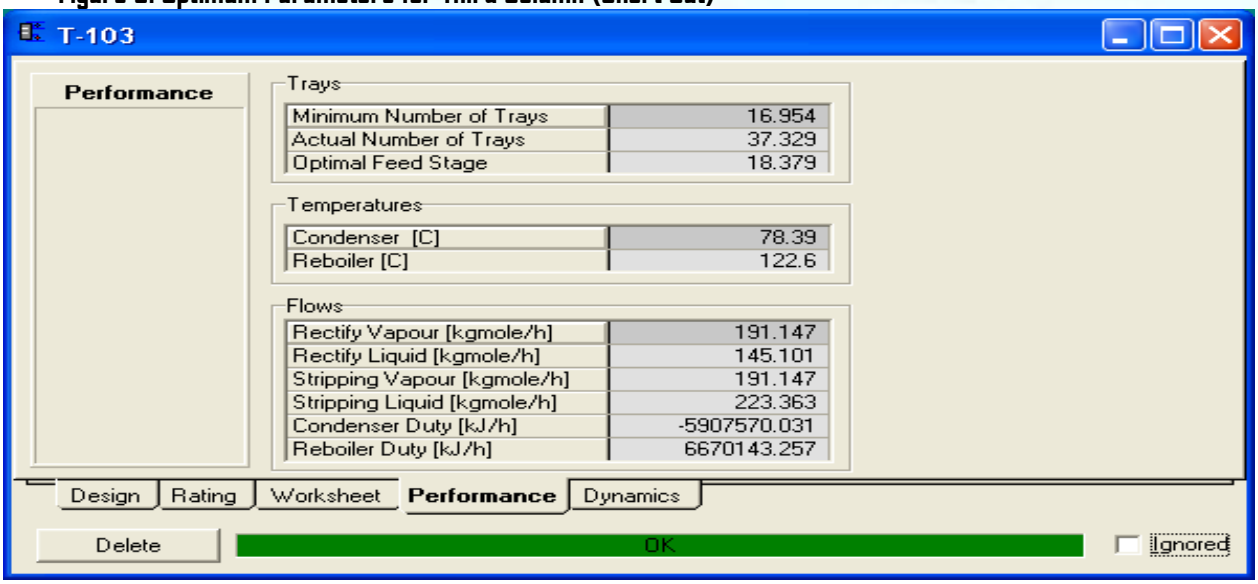


Figure 10: Optimum Performance for the Third Column

Table 8: data from Third column (Benzene as Product)

Benzene in Bottom, moles	n-heptanes in Distillate, mole	Actual No of Trays	Condenser duty KJ/hr	Reboiler Duty KJ/hr	Product Rate Kmol/hr	Benzene Purity, (%)	Ext Reflux ratio
0.0100	0.0100	41.0000	-6038071.8550	6801449.8410	46.1400	99.0000	3.2350
0.0200	0.0150	37.0000	-5907570.0310	6670143.2570	46.0500	98.5000	3.1550
0.0500	0.0500	26.0000	-5265044.2310	6002860.5820	46.7800	950.0000	2.6340

From the three columns designed in general, changing any parameter, component or performance of a column affected the performance of the next column (including the purity and flow rate of the products). Increase in reflux ratio and number of trays increased the purity of the products. Most columns are designed to operate between 1.2 to 1.5 times minimum reflux ratio (Tham, 1997; Chen and Lin, 2001; Luyben, 2013). So, to achieve a high level of purity with 1.2 times the minimum reflux ratio was a good demonstration of the strength of distillation process in separating aromatics. Also, it can be seen from the Hysys file that distillation process can be used to separate aromatics to achieve high level of purity, giving that the purity of benzene and toluene obtained in this study was very close to 99%.

In an earlier study, similar distillation process for separation of benzene, toluene xylene and C_9 components with tow sequential distillation column having total number of trays (77 + 70) equal to 147 trays and heating rate of 6.3* 10^7 KJ/h and cooling rate of 4.3*10^7KJ/h was reported to be feasible and economical by Masoumi and Kadkodaie (2012). Comparing the heating rate and the cooling rate of the distillation process in this study which were 24,935,057.21 KJ/h and -20,604,057.61 KJ/h respectively with heating rate and cooling rate of 6.3* 10^7 KJ/h and 4.3* 10^7 KJ/h respectively reported by Masoumi and Kadkodaie (2012), it can be reasonably argued that the distillation process was feasible and energy efficient. Furthermore, 1.2 to 1.5 times the minimum reflux ratio was approximately the region of minimum operating cost. More reflux means higher reboiler duty (Tham, 1997; Luyben, 2013). This distillation process was feasible because the numbers of trays and reflux ratio required to achieve high purity is within acceptable range in designing a distillation column. In addition, the process was energy efficient given that the heater and reboiler duty (24,935,057.21 KJ/h) and the condenser and cooler duty (-20,604,057.61 KJ/h) were within acceptable range and moreover, the energy generated can be recovered in form of steam that can be used within or somewhere.

Conclusion

It can be concluded that Aspen Hysys; selecting Wilson Fluid Package for physical properties of each components can be used to model distillation process which can obtain streams of toluene and benzene of high purity from reformate of catalytic cracking (or reforming) unit at high efficiency and low cost.

Recommendation

Purity of the products (benzene and toluene) can be improved with the same columns and the same number of trays under the same operating temperature and pressure by decreasing the mole fraction of the light key and heavy key in the bottom and distillate respectively and by increasing the reflux ratio by increasing the pump rate. Operating cost can be reduced by recovering the energy generated in form of steam which can be used within or supplied elsewhere to generate money thereby reducing the cost of energy to the process.

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