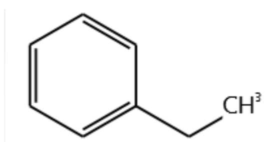
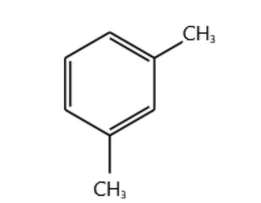
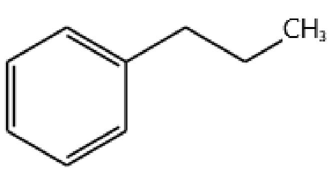
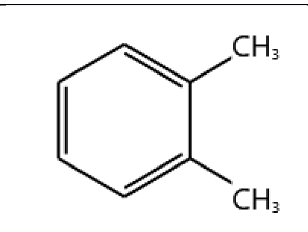
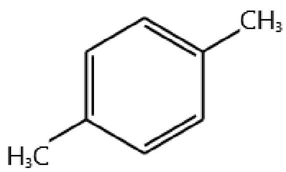
Solomon Leo

Aspen Project

CHE 363

Part A

Chemical Structure	Boiling Point at 1.5atm	Price
Ethylbenzene 	152C	$568/ton
p-xylene 	154.3C	$849/ ton
m-xylene 	154.9C	$420 / tonne
o-xylene	160.4C	$1460 / ton

		
n-propylbenzene 	175.8C	$1866/tonne

Each of the above chemicals are derived from petrochemical processes. Ethylbenzene is a byproduct of processing petroleum and is used as a solvent for some polymers such as styrene. It currently sells for $568/ton on the US market. It is also used in asphalt and synthetic rubbers. P-xylene is used as a feedstock to make TPA, PTA, and DMT which can be used to make plastics such as PET which is used in plastic bottles. It currently sells for $849/ ton on the US market. M-xylene is used primarily to produce isophthalic acid which is used in copolymerizing. It is widely used in dyes and rubbers. It currently sells for $420/ ton on the US market. O-xylene is used to produce phthalic acid which is used to produce many other drugs and chemicals. It currently sells for $1460/ ton on the US market. N-propylbenzene is used to dye textiles and to produce methyl styrene which is used to make plastics. It currently sells for $1866/ tonne on the US market.

The boiling points of the chemicals listed above are relatively close to each other which suggests that separating them will be difficult. N-propylbenzene has the most different boiling point which means that it will likely be the easiest to separate. If we want high recovery of ethylbenzene the closeness in boiling points will make it hard to separate from the xylenes meaning that we may need to run more columns or change the physical parameters inside them to separate.

Part B

In our first simulation we ran a DSTWU column with 20 plates with feed fed at the 10^{th} stage at a pressure of 1.5 atm. The process flow sheet can be seen below.

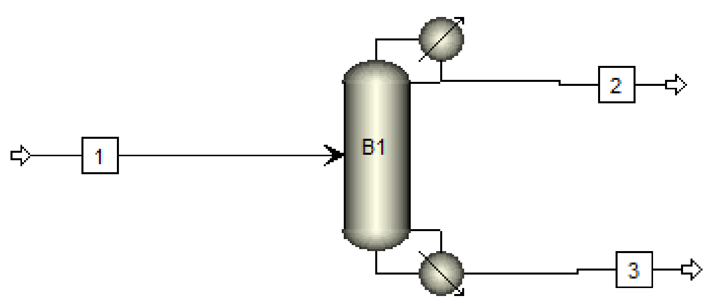


Figure 1: Process flow sheet for DSTWU column.

The molar flow rates and mol fractions can be seen below.

Table 1: Table of molar flow rates and temperatures for streams around column B1.

Component	SS (kmol/h)	6 (kmol/h)	S8 (kmol/h)
Ethylbenzene	47.5	34.88	12.62
p-xylene	211.64	144.72	66.92
M-xylene	446.78	307.65	139.13
o-xylene	170.48	87.74	82.74
N-propylbenzene	0.57	0.00114	0.57
Temperature (C)	155	115	115

Table 2: Table of mol fractions for streams around column B1.

Component	SS (mol%)	6 (mol%)	S8 (mol%)
Ethylbenzene	0.054	0.061	0.047
p-xylene	0.24	0.25	0.22
M-xylene	0.51	0.53	0.46
o-xylene	0.19	0.15	0.27
N-propylbenzene	0.00065	1.97e-6	0.0019

Table 3: Table of number of actual stages, minimum stages, minimum reflux ratio, and feed stage for column B1.

Number of actual stages	20
Minimum number of stages	10.16
Minimum reflux ratio	1.35
Feed stage	10.74

Part C

In our next simulation we ran a RadFrac column with 20 plates at 1.5 atm with the feed stage at stage 10. The process flow sheet is shown below.

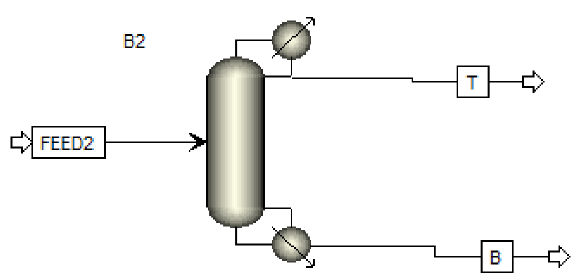


Figure 2: Process flow sheet for RadFrac column.

Table 4: Table of molar flow rates and temperatures for streams around RadFrac column.

Component	FEED2 (kmol/h)	T (kmol/h)	B (kmol/h)
Ethylbenzene	50	0.5	50
p-xylene	231	4.54	226.45
M-xylene	483	7.44	475.53
o-xylene	222	18.28	203.72
N-propylbenzene	14	13.51	0.48
Temperature (C)	150	162.11	155.09

Table 5: Table of mol fractions for streams around RadFrac column.

Component	FEED2 (mol%)	T (mol%)	B (mol%)
Ethylbenzene	0.05	0.011	0.052
p-xylene	0.231	0.10	0.23
M-xylene	0.438	0.17	0.49
o-xylene	0.222	0.14	0.21
N-propylbenzene	0.014	0.31	0.00051

Table 6: Table of number of stages and feed stage for RadFrac column.

Number of actual stages	20

Feed Stage	10

To reach 99% recovery of the light key, and 3.5% of the heavy key, we set the column to a pressure of 1.5 atm and manipulated the reflux ratio of the column. At higher reflux ratios, we can achieve higher recovery. This can be seen in the specification tables where the DSTWU had a reflux ratio of 1.6 and the RadFrac had a reflux ratio of 3.12 which is almost double the DSTWU. This increased reflux ratio results in an increased heat and cooling duty for the reboiler and condenser leading to a higher cost to operate. The set number of stages was 20 with the feed stage at stage 10 and we had a reasonable reflux ratio meaning that this process is feasible to run. It had the same number of stages as the DSTWU in Part B.

Part D

Finally to separate two streams of at least 0.9 mol% purity, we connected two RadFrac columns in series to the top of the DSTWU shown in Part A. These RadFrac columns were run at 0.5 atm and the specifications can be seen below. We also connected a DSTWU to the bottom of the initial DSTWU from Part A at a pressure of 0.5 atm. The process flow sheet can be seen below.

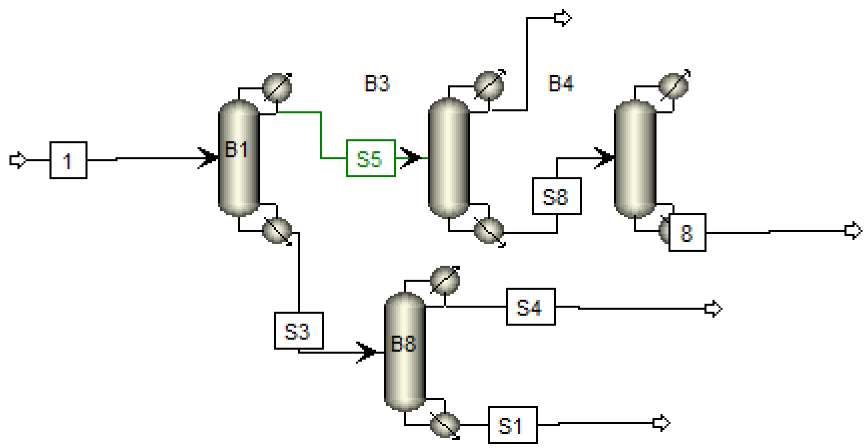


Figure 3: Process flow sheet to obtain two streams with at least 90% purity.

The operating parameters and stream results can be seen in **Table 1** to **Table 3** since B1 is the same as the DSTWU column in Part B.

B3 (RadFrac)

Table 7: Table of molar flow rates and temperatures for streams around column B3.

Component	S5 (kmol/h)	6 (kmol/h)	S8 (kmol/h)
Ethylbenzene	47.5	34.88	12.62
p-xylene	211.64	144.72	66.91
M-xylene	446.78	307.65	139.13
o-xylene	170.48	87.77	82.74

N-propylbenzene	0.57	0.0011	0.57
Temperature (C)	155	114.97	114.65

Table 8: Table of mol fractions for streams around column B3.

Component	S5 (mol%)	6 (mol%)	S8 (mol%)
Ethylbenzene	0.054	0.061	0.042
p-xylene	0.241	0.25	0.22
M-xylene	0.509	0.54	0.46
o-xylene	0.194	0.15	0.27
N-propylbenzene	0.00065	1.98e-6	0.0019

Table 9: Table of number of stages and feed stage for column B3.

Number of actual stages	20
Feed Stage	10

B4 (RadFrac) (feed stage: 25, stages 50)

Table 10: Table of molar flow rates and temperatures for streams around column B3.

Component	S8 (kmol/h)	8 (kmol/h)	S2 (kmol/h)
Ethylbenzene	12.61	0.078	12.54
p-xylene	66.89	2.51	64.39
M-xylene	139.04	2.01	137.03
o-xylene	82.65	46.59	36.05
N-propylbenzene	0.57	0.57	2.62e-6
Temperature (C)	115.65	118.98	114.96

Table 11: Table of mol fractions for streams around column B3.

Component	S8 (mol%)	8 (mol%)	S2 (mol%)
Ethylbenzene	0.042	0.0015	0.05
p-xylene	0.22	0.048	0.26
M-xylene	0.46	0.039	0.55
o-xylene	0.27	0.9	0.14
N-propylbenzene	0.0019	0.011	1.05e-8

Table 12: Table of number of stages and feed stage for column B3.

Number of actual stages	50
Feed Stage	25

B8 (DSTWU)

Table 13: Table of molar flow rates and temperatures for streams around column B1.

Component	S3 (kmol/h)	S1 (kmol/h)	S4 (kmol/h)
Ethylbenzene	2.5	0.00067	2.49
p-xylene	19.35	0.018	19.33
M-xylene	36.32	0.033	36.29
o-xylene	51.62	0.52	51.11
N-propylbenzene	13.43	12.89	0.54
Temperature (C)	158.19	132.80	116.62

Table 14: Table of mol fractions for streams around column B1.

Component	S3 (mol%)	S1 (mol%)	S4 (mol%)
Ethylbenzene	0.02	4.98e-5	0.023
p-xylene	0.16	0.0013	0.18

M-xylene	0.29	0.0025	0.33
o-xylene	0.41	0.038	0.47
N-propylbenzene	0.11	0.96	0.0049

Table 15: Table of number of actual stages, minimum stages, minimum reflux ratio, and feed stage for column B1.

Number of actual stages	20
Minimum number of stages	16.91
Minimum reflux ratio	1.54
Feed stage	9

We cannot fully separate all of these components since their boiling points are very similar. This makes this mixture very difficult to separate since it will only flash in a small region making distillation especially difficult. To increase the range of the two phase region and extract lighter components, we chose to reduce the pressure of the new columns (B3, B4, B8) to 0.5 atm from 1.5 atm. In terms of feasibility, the reflux ratio of the columns are all reasonable since they are below 10. The only column that raises some feasibility concerns is B4 since it has 50 stages. Typically the columns should be around 20 stages. One change would be to run two smaller columns in series rather than one big column. We could sell these higher purity streams at higher prices increasing the revenue for the plant. Some environmental concerns would be leaks from the columns or piping between the columns. With more columns we have more points of failure for the process which could lead to more frequent accidents or spills. The same applies for overall safety concerns.