Process Simulation of 1-Butene and N-Butane Separation By Extractive Distillation

M. Naeem[1], A. A. Al-Rabiah[2] and W. Mughees[3]
Master Student, Chemical Engineering Department, Kind Saud University, Riyadh, Saudi Arabia[1]
Assistant Professor, Chemical Engineering Department, Kind Saud University, Riyadh, Saudi Arabia[2]
Master Student, Chemical Engineering Department, Kind Saud University, Riyadh, Saudi Arabia[3]

***Abstract*— Technical mixture of C4 containing 1-butene and n-butane are very close to each other w.r.t. their boiling points i.e. -6.3°C for 1-butene and -1°C for n-butane. Extractive distillation process is used for the separation of 1-butene from the existing mixture of C4. The solvent is the essential of extractive distillation, and an appropriate solvent shows an important role in the process economy of extractive distillation. Aspen Plus has been applied for the separation of these hydrocarbons as a simulator; moreover NRTL activity coefficient model was used in the simulation. This model indicated that the material balances in this separation process were accurate for several solvent flow rates. Mixture of acetonitrile and water used as a solvent and 99 % pure 1-butene was separated. This simulation proposed the ratio of the feed to solvent as 1 : 7.9 and 15 plates for the solvent recovery column, previously feed to solvent ratio was more than this and the proposed plates were 30, which can economize the separation process.**

Keywords— Extractive distillation, 1-butene, Aspen Plus, ACN solvent.

I. INTRODUCTION

Hydrocarbons having very close boiling points are mostly separated by extractive distillation, for example the mixtures of C4's, C5's and C6's and more [1]-[3]. This type of hydrocarbon separation needs very high reflux ratio and number of trays [4].

Extractive distillation always needs a potential solvent, and an appropriate solvent shows a significant role in the economical design of extractive distillation [5]-[7]. In extractive distillation, an additional solvent as a separating agent is used to change the relative volatility of the components required to be separated. With this method, one pure component is achieved at the top of the first column and the second component goes with the solvent at the bottom of the same column in the residue, which may then be easily separated in a secondary distillation column because of the high boiling point of the solvent and lower boiling point of the component to be separated [8]-[11].

While producing ethylene and propylene by pyrolysis of liquefied petroleum gas or naphtha, C4 mixtures are produced. Generally, C4 mixtures mainly contain n-butane, isobutane, isobutene, 1-butene, trans-2-butene, cis-2-butene, 1,3-butadiene, and vinylacetylene. Previously, scientists paid more attention in the production of 1,3-butadiene, which is very important raw material from this kind of mixtures [12]. However, among the residue, n-butene (that is, the mixture of 1-butene, trans-2-butene, and cis-2-butene) is able to be used as one monomer of producing polymers and one reactant of producing acetone by reacting with water. Isobutene can be selectively combined with methanol to make methyl tert-butyl ether (MTBE) [12]. Unluckily, the separation of butane and butene has rarely been studied. Therefore, extractive distillation is here used for the separation of butane and butene using a suitable solvent for this purpose. The first possible solvent can be the combination of acetonitrile (ACN) with Ethylenediamine which are completely miscible, and then the second potential solvent can be the mixture of ACN and water, thirdly the potential solvent can be ACN alone. All three cases have been examined in our simulating model but most high results obtained using ACN with water as a solvent.

In this paper, an approach has been adopted to determine the minimum solvent to feed ratio, minimum number of trays for the second distillation column. Aspen Plus has been used to carry out the required objectives. The results of this work are more precise than the referred previous work discussed in the literature.

II. PROCESS DESCRIPTION

Process simulation of the separation of n-butane and 1-butene by extractive distillation with the mixture of ACN with water as the solvent was performed using Aspen Plus version 11.1. This process consisted of 70 theoretical plates of the first extractive distillation column and 15 theoretical plates for the solvent recovery column. The feeding mixture was composed of 20 wt. % n-butane and 80 wt. % of 1-butene with a total flow rate of 2450 kg/h, and the feed/solvent mass ratio was 1 : 7.918. Table shows the feed composition.

TABLE 1

	Component	Mass (wt. %)
Composition of feed	n-butane	20
	1-butene	80

The extractive distillation column was operated at the top pressure of 450 kPa and the bottom pressure of 630 kPa. Reflux ratio was set at 5.0, n-butane is the distillate of this column at the rate of 490 kg/hr. Feed stream was fed above the stage number 40 and solvent was fed to the column above the stage number 5. Working conditions of the solvent recovery column are somehow different. This column operated at top pressure 200 kPa and the bottom pressure of 260 kPa with the reflux ratio 4.0. Bottom exit stream of extractive distillation column enters above stage number 10 into the solvent recovery column. Therefore, distillate of the solvent recovery column is 99 % pure 1-butene and the downstream is ACN and water mixture as solvent which is partially recycled to the first column to make the plant efficient w.r.t. economy. Table below shows the configurations of both the columns used in our simulation.

TABLE 2

	Configurations	Extractive Distillation Column	Solvent Recovery Column
Configuration of distillation columns	Top pressure	450 KPa	200 KPa
	Bottom pressure	630 KPa	260 KPa
	Number of trays	70	15
	Reflux ratio	5	4
	Feed tray	40	10
	Solvent feed tray	5	Nil

Our simulated work is different as previously done by using Pro II. Previously mixture of ACN with water and ACN with ethylenediamine as solvents were studied, moreover, 30 theoretical plates for the solvent recovery column were reported. However, in this work, Aspen Plus is used as a simulator and only 15 theoretical plates are reported for the solvent recovery column using only ACN and water as solvent, which is the great achievement. Feed to solvent ratio was proposed 1:10 which was too much high, this work reports only 1 : 7.918. Another major difference was the composition of the feed mixture, in which 1-butene was already 93.9 % pure by weight [12] in the previous work; our proposed work used the feed mixture of 80 % 1-butene and 20 % n-butane. Therefore, it is the new and economical innovation for the purification of the 1-butene.

In this part of our work we will try to present the simulated work using flow sheet and the results which we got from the software. Therefore, shown figure # 1 consist of two columns and one mixer and one splitter, operating conditions of these units are already discussed, however this figure may help to explain the process in a very simple way. As shown in the figure there are total 9 streams, each of which has different composition as shown in the figure # 2. Stream 1 containing solvent Acetonitrile (ACN) and water enters in the mixer then stream 2 exiting from mixer is going to enter in the first column know as extractive distillation column. Stream 3 is our basic feed comprising of 20% n-butane and 80% 1-butene. This column works under the circumstances of a set of provided working conditions and expels two streams, stream 4 contains n-butane (may contain some of the 1-butene and ACN with water) as a distillate of this column. Stream 5 majorly consists of 1-butene and solvent and enters to the second column which here is known as solvent recovery column. As shown that, our key component stream 6 contains 1-butene which is 99% pure as the distillate. Stream 7 consists of almost pure solvent enters to the splitter where some of the solvent sent back to the mixer as recycle.

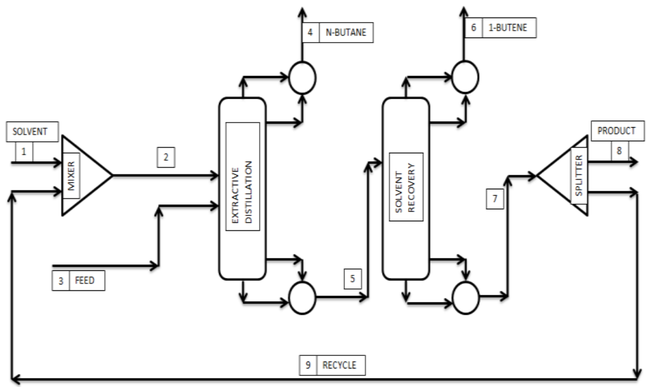

Fig. 1 Process overview

TABLE 3

Mole fractions	Streams								
	1	2	3	4	5	6	7	8	9
n-butane	0.0	1.05E-11	0.20	0.92	3.43E-04	7.69E-03	1.04E-10	1.04E-10	1.04E-10
1-butene	0.0	4.05E-05	0.80	5.91E-04	0.044	0.992	4.05E-04	4.05E-04	4.05E-04
Acetonitrile	0.80	0.80	0.0	0.013	0.762	7.25E-05	0.798	0.798	0.798
Water	0.20	0.20	0.0	0.065	0.192	7.22E-06	0.201	0.201	0.201

Table # 3 shows the mass balance which gives the details of all the stream compositions from stream 1 to last i.e. stream 9. If we see this table and process sheet together then we came to know that stream 4 and stream 6 are of our major concern which are distillate of extractive distillation column and solvent recovery column respectively. Therefore due to our objective we can highlight these two streams to view full results obtained from the simulator.

III. RESULTS AND DISCUSSION

This table clears each and every thing to us about the stream 4. n-butane is our distillate in this stream and we can see in this stream table that major composition is of n-butane. Mole flow, mole fraction, mass flow and mass fraction all verifies the purity of n-butane. Therefore, purity reaches to 96 % by weight which is highly admirable. Similarly, next table shows the purity of 1-butene i.e. 99 % by weight. Similar results can be seen in the table form shown below.

TABLE 4

	Component	Mass (wt. %)
Composition of product	n-butane	96
	1-butene	99

Finally we got good separation results from C4 mixture applying simulation on whole unit by using previously discussed set of conditions and parameters.

TABLE 5

	Flow and fractions	Value
Results of stream # 4	Mole flow lbmol/hr	
	n-butane	17.894
	1-butene	0.127
	ACN	0.247
	Water	1.270
	Mole fraction	
	n-butane	0.915
	1-butene	0.006
	ACN	0.012
	Water	0.065
	Mass flow lb/hr	
	n-butane	1040.075
	1-butene	7.152
	ACN	10.152
	Water	22.884
	Mass fraction	
	n-butane	0.962
	1-butene	0.006
	ACN	0.009
	Water	0.021
	Total flow lbmol/hr	19.539
	Total flow lb/hr	1080.265

Above table is the description of simulated results of stream # 4 coming out from the first extractive distillation column as distillate from the top of the column. Similarly, Table V shows the complete description for the stream # 6. This stream is the distillate of the second distillation column giving 99 % pure 1-butene.

TABLE 6

	Flow and fractions	Value
Results of stream # 6	Mole flow lbmol/hr	
	n-butane	0.691
	1-butene	76.302
	ACN	0.005
	Water	0.000
	Mole fraction	
	n-butane	0.008
	1-butene	0.990
	ACN	0.000
	Water	0.000
	Mass flow lb/hr	
	n-butane	40.168
	1-butene	4281.146
	ACN	0.236
	Water	0.010
	Mass fraction	
	n-butane	0.009
	1-butene	0.990
	ACN	0.000
	Water	0.000
	Total flow lbmol/hr	77
	Total flow lb/hr	4321.562

Presented graphical trends are showing the dependency of purity of the 1-butene on reflux ratios and the solvent to feed ratio. Figure 2 shows the relation between reflux ratio and purity of 1-butene in the extraction distillation column. It is obvious from the figure that, increase in the reflux ratio caused purity increase up to some value, after that purity does not increase.

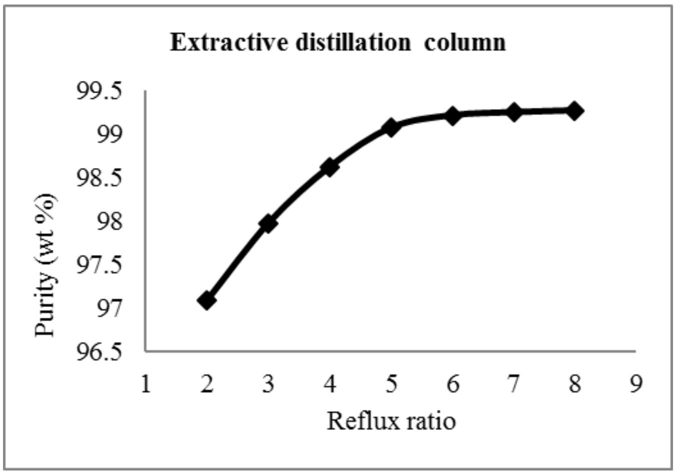

Fig. 2 Purity of 1-butene due to reflux change in extractive distillation column

Similarly, Figure 3 represents the relation between reflux and the purity in the solvent recovery column.

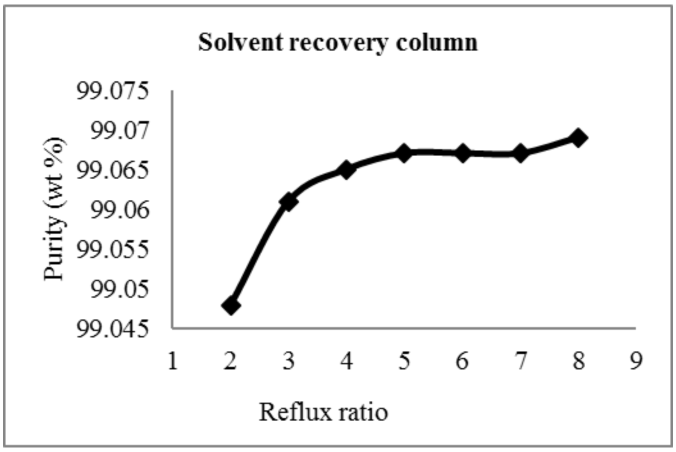

Fig. 3 Purity of 1-butene due to reflux change in solvent recovery column

Most important relation is shown in figure 4, It represents that for the purity of 99% pure 1-butene, solvent to feed ratio up to 1 : 7.9 is best value.

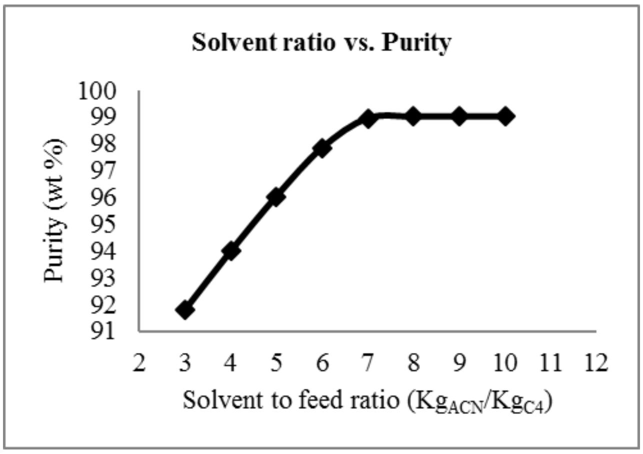

Fig. 4 Purity of 1-butene due to solvent to feed ratio

IV. CONCLUSION

Aspen Plus was used as a simulator to perform distillation processes for the separation of 1-butene and n-butane. Thermodynamic properties were calculated using NRTL as activity coefficient model. 99 % pure 1-butene was separated from the C4 mixture consisting 20% n-butane and 80% 1-butene. This work reports less solvent to feed ratio and only 15 plates for the second distillation column. Therefore, these simulation results can be used to reduce the process cost.

ACKNOWLEDGMENT

Authors are grateful to the Deanship of Scientific Research Centre at College of Engineering, King Saud University (KSU), which rendered technical support in this study.

REFERENCES

[1] L. Berg, "Separation of benzene and toluene from close boiling nanoramactics by extractive distillation" AIChE. J., Vol. 29, pp. 961–966, 1983.
[2] B. Chen, Z. Lei, J. Li, "Separation on aromatics and non-aromatics by extractive distillation with NMP" J. Chem Eng Jpn., Vol. 36, pp. 20-24, 2003.
[3] Z. Lei, C. Li, B. Chen, "Extractive distillation: A review" Sep Purif Rev. Vol. 32, pp. 121-213, 2003.
[4] K. YoungHoom, K. SungYoung, L. Bomsock, "Simulation of 1,3-butadiene extractive distillation process using N-methyl-2-pyrrolidone solvent" Korean J. Chem Eng., Vol. 29, pp. 1493-1499, 2012.
[5] KG. Joback, G. Stephanopoulos, "Searching spaces of discrete solutions: The design of molecules possessing desired physical properties" Adv Chem Eng., Vol. 21, pp. 257-311, 1995.
[6] V. Venkatasubramanian, K. Chan, JM. Caruthers, "Generic algorithmic approach for computer-aided molecular design" ACS Symp Ser., Vol. 589, pp. 396-414, 1995.
[7] N. Churi, LEK. Achenie, "Novel mathematical programming model for computer aided molecular design" Ind Eng Chem Res., Vol. 53, pp. 3788-3794, 1996.
[8] EC. Marcoulaki, AC. Kokossis, "Molecular design systhesis using stochastic optimization as a tool for scoping and screening" Comput Chem Eng., Vol. 22, pp. S11-S18, 1998.
[9] ML. Mavrovouniotis, "Design of chemical compounds" Comput Chem Eng., Vol 22, pp. 713-715, 1998.
[10] AH. Meniai, DMT Newsham, B. Khalfaoui, "Solvent design for liquid extraction ysing calculated molecular interaction parameters" Chem Eng Res Des., Vol. 76, pp. 942-950, 1998.
[11] JE. Ourique, AS. Telles, "Computer-aided molecular design with simulated annealing and molecular graphs" Comput Chem Eng., Vol 22, pp. S615-S618, 1998
[12] C. Biaohua, L. Zhigang, L. Qunsheng, L. Chengyue, "Application of CAMD in separating hydrocarbons by extractive distillation" AIChE J. Vol. 51, No. 12, pp. 3114-3121, 2005.