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Modelling and Optimization of PSA (Pressure Swing Adsorption) Unit by using Aspen Plus® and Design Expert ®

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Abstract: ***Pressure swing adsorption (PSA) is a well-established technique for separation of components from air, which is commonly known as Air Separation Unit (ASU), drying of gas and nitrogen and hydrogen purification separation and etc. In PSA processes, the most important is adsorbent material depending upon its properties. Generally, ASU is difficult to operate due to high degree of energy integration into itself. This research article represents the separation of nitrogen from air. As separation of nitrogen is a very important in the field of chemical engineering as it has wide applications in the various process industries. There are various techniques for separation of nitrogen, amongst them the most common are reverse stirling cycle, LINDE-HAMPSON cycle, Joule Thompson effect and etc. This article mainly focusses on the separation of nitrogen using PSA unit only. The whole process was simulated using Aspen Plus ® and the simulated results were then optimized using Design Expert ®. Various flowrates ranging from 50 kg/h to 200 kg/h were selected, depending upon the process conditions. The output of the simulated results from Aspen Plus ® were then optimized using Box Behnken method, in order to obtain the optimized flowrate of Nitrogen. The response pattern suggest that the flowrates of nitrogen and other gases follows quadratic equation. The significance of the coefficients of the equation and the adequacy of the fit were determined using Student-t test and Fischer F-test respectively. The final flowrates obtained are interchanged in order to obtain the maximum conditions, except for nitrogen production other production rates remain the same.***

Index Terms: ***Nitrogen, PSA (pressure swing Adsorption), Aspen Plus®, Design Expert®.***

I. INTRODUCTION

Air is a composition of various gases, of which nitrogen (N_2) and oxygen (O_2) are the main components and apart from that there are other gases, which are present in the air in trace amount. According to the previous researchers Liu. et. al., oxygen and nitrogen are used most extensively by various industries [1]-[2]. Generally, nitrogen is used in chemical, petroleum, food, pharmaceutical and nuclear and etc., whereas oxygen is used by petroleum refineries, medical, concrete and wielding industries, chemical and gasification and etc. and other gases are used in steel making, heat treatment, manufacturing process for electronics and etc. Because of the different demand for the gas purity, gas amount and gas usage, there are two different types of air separation unit (typically 75 ~ 105%). If a lower volume, gaseous oxygen or nitrogen product is required, then pressure swing adsorption [2] and membrane separation [3] may be used or else larger volume of gaseous products, high purity products or the recovery of argon, cryogenic air separation processes will be used [2], which is operated at extremely low temperature (-170^{o}C~- 195^{O}C). Cryogenic air separation unit processes separate air components according to their different boiling temperatures [4]. Nowadays membrane processes like molecular sieves are gaining importance. As membrane units are capable of producing nearly 600 tonnes of nitrogen per day, having a purity of 90-99%. Commonly used molecular sieves are carbon molecular sieves [CMS] [15].

This paper represents the process design of air separation unit process using Aspen Plus ®, computer based simulation, for different chemical engineering purposes. Our aim was to calculate the production of N_2. Various flowrates ranging from 50 kg/h to 200 kg/h were selected, depending upon the process conditions. The output of the simulated results from Aspen Plus ® were then optimized, in order to obtain the optimized flowrate of Nitrogen using Design Expert ®. Though the design calculation does not give the real-life production environment but it can provide relief from making wide range of experiment without making the small-scale reactor or plant.

II. METHODOLOGY

The whole system was simulated using Aspen Plus ®, which is shown in the figure 1. and then the sensitivity of the final flowrates of N2 and other gases, from the computer-based simulation were optimized using Design Expert ®.

II. A. ASPEN PLUS MODELLING

Aspen Plus ® has been used for the separation of Nitrogen from atmospheric air, as it provides accurate results compared to the real life [5]. Depending on the comprehensive thermodynamics' properties, based on physical properties [8], transport properties and phase behavior [6]. The present simulation used Ideal and Peng-Robinson models which fits best to equilibrium since components are gaseous and non-polar. The components used are N2 (non-polar) and O2 (non-polar) for simplicity. Figure 1. shows the PSA of the process of separation of nitrogen from air.

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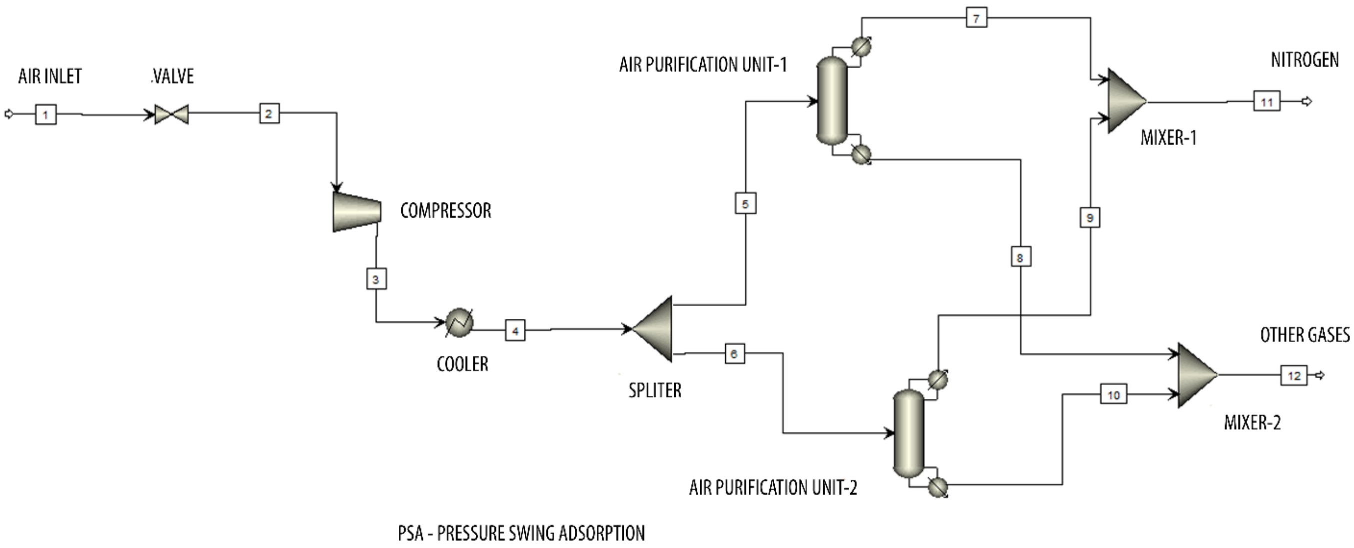

Figure 1. Process block diagram of the process of separation of separation of nitrogen from air.

Process Description:

Generally atmospheric air contains dust. So for this reason air is needed to be purified, but in our simulation we had considered dust free air which is mainly composed of nitrogen, oxygen and small traces of water vapor. Initially, for the simulation we had considered flowrates varying from 50kg/h to 200 kg/h and temperature variation from 298K to 313K and pressure of 7e-7bar and the mass fraction of air constituted of nitrogen-77%, oxygen-20% and water vapor-3%.

The gas stream passes through valve, (J-T valve), before entering into compressor. The compressor type used during simulation is Polytropic using GPSA method and with a discharge pressure of 5 bar. After passing through the compressor, the gas stream enters into cooler where the temperature is maintained at 298K.

The output of the cooler is spitted and enters into purification unit 1 and 2, where the number of stages, condenser, reboiler, valid phase, distillate rate and reflux ratio are selected and the results are 33, total, kettle, vapor-liquid, 5.88e-7 kmol/sec and 0.75 respectively. The final output gases product are nitrogen and other gases (oxygen and water vapor). The detailed description of the process parameters is provided in the table A5.

III. PARAMETRIC SENSITIVITY AND OPTIMIZATION

The effects of parameters namely, temperature (T) and air flowrate (a) of air are the major response variables namely, A and B have been correlated mathematically. The model equations have been developed with the aid of response surface methodology [10] simultaneously varying the values of f and T. The values of (T) and (a) were fixed using Box Behnken method [11,12].

The mathematical relationships between the responses (Yi) and factors, air flowrates (X1) and temperature (X2) are given by,

$$Y_i = f_i(X_1, X_2) \text{ where } i = 1, 2 \qquad (1)$$

Y_1 = air flowrates
Y_2 = temperature

It is assumed that the independent factors A and B are continuous and controllable by experiments with negligible errors. The generalized second order polynomial, correlating the responses with the independent factors, is of the following form:

$$y_i = \alpha_i + \sum_{j=1}^{2} \beta_{ij} X_j + \sum_{j=1}^{2} \sum_{\substack{u=1 \\ u \neq j}}^{2} \beta_{iuj} X_u X_j + \sum_{j=1}^{2} \beta_{ijj} X_j^2$$

The significance of the coefficients and the adequacy of the fit are determined using Student-t test and Fischer F-test respectively. The values of Nitrogen flowrates and other gases flowrates (oxygen and water) respectively have been maximized and minimized. The development of model equation and optimization has been done using Design -Expert Software 7.0 ® [9].

IV. RESULTS AND DISCUSSION

After performing the simulation, we had observed that the production of nitrogen is maximum, as compared to the other gases, which were considered during the simulation. The final flowrates obtained from Aspen Plus ® are shown in the figure 2 and figure 3. It is clearly evident from figure 2 that the flowrates of nitrogen continuously increase as the flowrates of air increases. The detailed production rates are provided in the table A4. Therefore, we can confirm that final composition of nitrogen varies from 76.8% to 77%. But

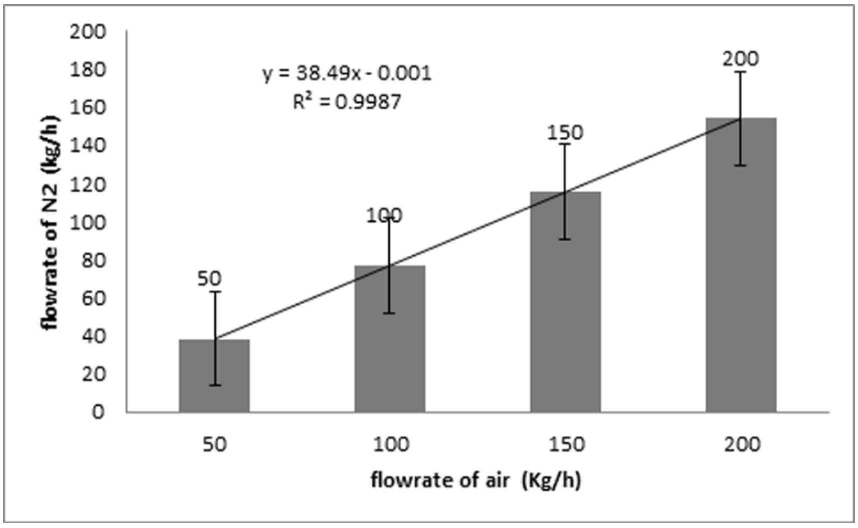

Figure 2. The flowrates of nitrogen with respect of inlet air.

this value is expected to be around 99%. The deviation in the result happened due to the unavailability of process conditions. The final flowrates of oxygen (figure 3.a) and flowrates of water (figure 3.b.) are represented below. It is evident from the figures that the flowrates of oxygen and water, which is the main composition of other gases, decreases when the flowrates of air increases from 50 kg/h to 100 kg/h. After which, as the flowrates of air increases the decrease in the production of oxygen and water decreases minorly. Thus it is confirmed that the production of nitrogen increases as the flowrates of air increases, whereas for other gases as the air flowrates increases the production rates decreases.

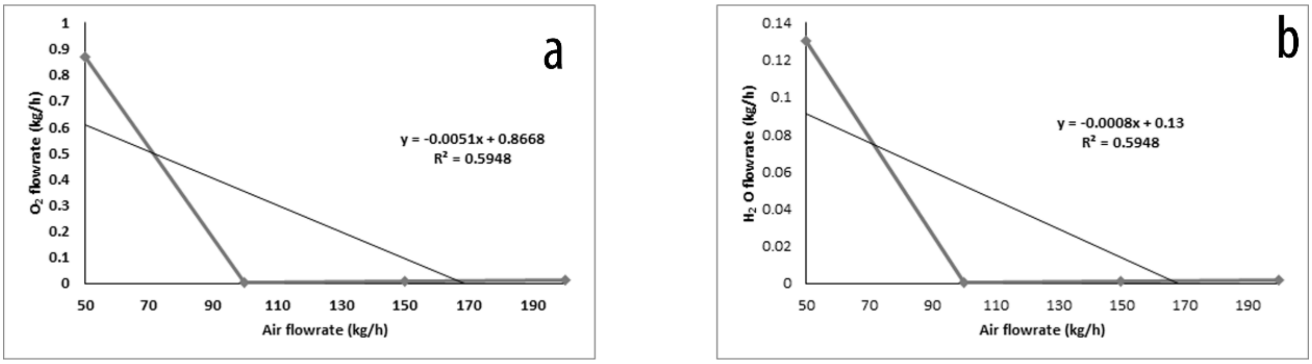

Figure 3. The flowrates of oxygen outlet with respect of inlet air. b. The flowrates of water outlet with respect of inlet air

Optimized flowrates output and Parametric Sensitivity.
The flowrates of nitrogen obtained varying flowrates and temperature are considered for calculating the optimization condition using response surface methodology. Design Expert® software had been used for this purpose. The quadratic equations obtained, which is predicted by the statistical modelling are as follows

$$y_i = \alpha_i + \sum_{j=1}^{2} \beta_{ij} X_j + \sum_{j=1}^{2}\sum_{u=1}^{2} \beta_{iuj} X_u X_j + \sum_{j=1}^{2} \beta_{ijj} X_j^2 \quad (1)$$

$$u \neq j$$

Figure 4 and figure 5 shows the flowrates of nitrogen and other gases (oxygen and water vapor) as a function of temperature and air inlet. From the ANOVA tables provided in the Appendix A1.-A3. The model equation obtained represents a surface quadratic type, indicating flowrates of nitrogen and other gases are dependent variable.

The model equation for optimum nitrogen flowrates is

$$\begin{aligned} f_{nitrogen} = {} & 11.74090 - 1.28473\text{e}^{-3} * (a) - \\ & 0.076555 * (T) + \\ & 6.25927e^{-6} * (a) * (T) \\ & - 2.34918e^{-6} * (a)^2 + \\ & 1.24563e^{-4} * (T)^2 \end{aligned} \quad (2)$$

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The model equations for optimum other gases (oxygen and water vapor) flowrates are

$$f_{oxygen} = -21.39390 - 0.02383*(a) + 0.15209*(T) - 8.4443e^{-6}*(a)*(T) + 8.11448e^{-6}*(a)^{2} + 2.46624e^{-4}*(T)^{2} \qquad (3)$$

$$f_{water\ vapor} = -4.92826 - 2.36966e^{-3}*(a) + 0.033509*(T) + 4.857785e^{-6}*(a)*(T) + 1.18665e^{-5}*(a)^{2} + 5.36769e^{-5}*(T)^{2} \qquad (4)$$

The maximum results for the flowrates of nitrogen (87.2136 kg/h), oxygen (140.608 kg/h) and water vapor (107.62 kg/h) have been obtained at T = 301.75K, 312.34K and 299.34K and a = 124.55 kg/h, 183.25 kg/h and 82.36 kg/h respectively. As predicted by the model equations 2-4, the optimum simulated results of nitrogen, oxygen and water vapor were interchangeable. Then nitrogen flow rate remained at 104.19 kg/h when the optimum operating condition for the maximum oxygen production was maintained. Therefore, interchanging the conditions in the above equations, except for nitrogen production others remains almost constant, which proves that at 104.19 kg/h the process is sensitive.

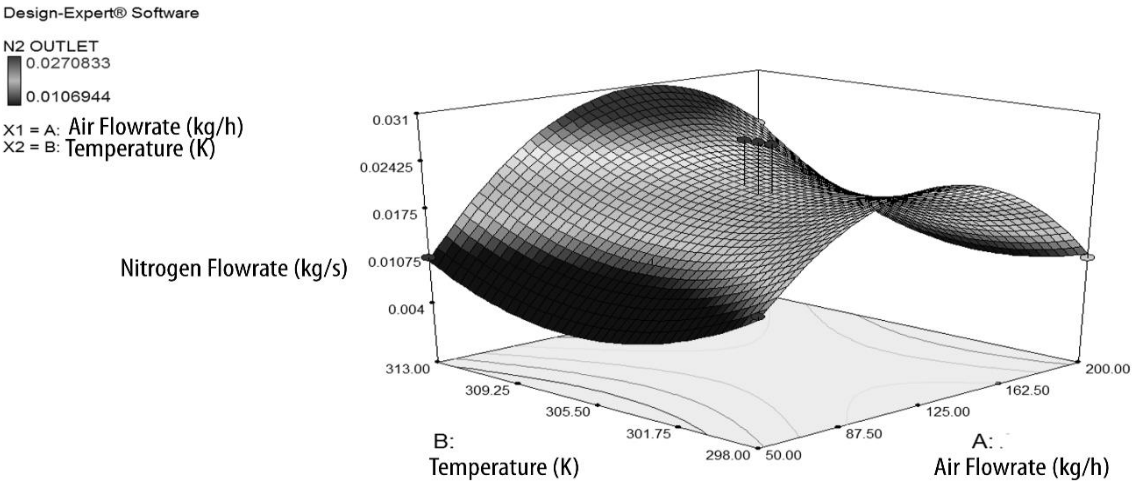

Figure 4. The flowrates of nitrogen as a function of temperature and air flowrates.

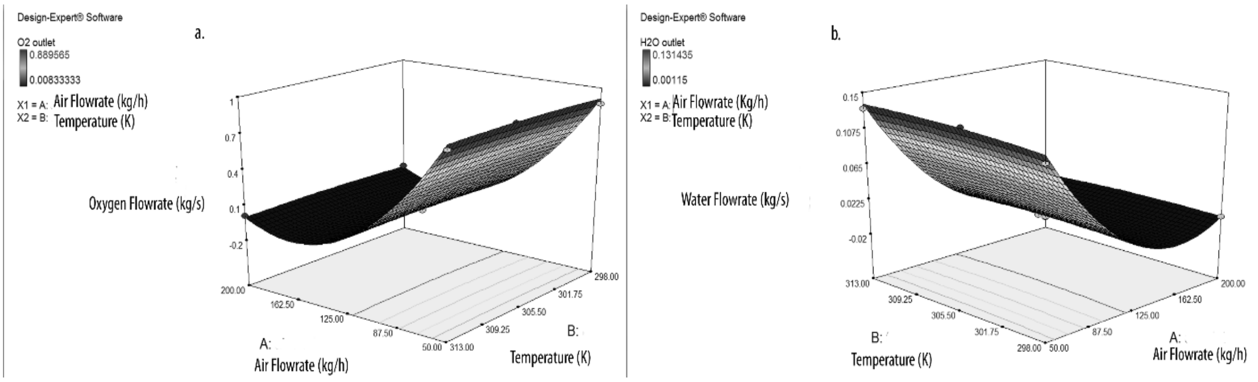

Figure 5. a. The flowrates of oxygen as a function of temperature and air flowrates. b. The flowrates of water vapor as a function of temperature and air flowrates.

IV. RECOMMENDATION FOR FUTURE SCOPE

Demand of nitrogen and oxygen are increasing from time to time. To meet this demand many industries especially chemical industries, refrigeration, air conditioning, nuclear and etc., established their own separate unit. In order to separate nitrogen from common source like ambient air. Simply PSA (pressure swing adsorption), which is a membrane based operation, is the most common and basic process of separation of nitrogen from ambient air.

This paper demonstrates the optimized flowrates of nitrogen using various process conditions. The process simulation software used for simulating the results is Aspen Plus® and the optimization of the process is carried out by Design Expert ®. The maximum optimized results for the flowrates of nitrogen (87.2136 kg/h),

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oxygen (140.608 kg/h) and water vapor (107.62 kg/h) had been obtained at T = 301.75K, 312.34K and 299.34K and a = 124.55 kg/h, 183.25 kg/h and 82.36 kg/h respectively. As, the optimum simulated results of nitrogen, oxygen and water vapor were interchangeable, then nitrogen flow rate remained at 104.19 kg/h when the optimum operating condition for the maximum oxygen production was maintained. Therefore, interchanging the conditions, except for nitrogen production others remains almost constant, which proves that at 104.19 kg/h the process is sensitive. So, there is a huge scope lies in the improvement and simulation of the process, but the process lacks energy exchange with surroundings. So advancement must be taken in the forward direction for the betterment of the process.

APPENDIX

A1. ANOVA for response surface quadratic model for the flowrate of nitrogen as a function of temperature and flowrate of air

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob < F	
Model	2.867E-004	5	5.734E-005	1.01	<0.4746	significant
A-AIRINLET	*4.376E-005*	1	*4.376E-005*	*0.77*	0.4081	
B-temp	*2.534E-005*	1	*2.534E-005*	*0.45*	0.5246	
AB	*4.959E-005*	1	*4.959E-005*	*0.88*	0.3801	
A^2	*1.537E-004*	1	*1.537E-004*	*2.72*	0.1431	
B^2	*4.145E-005*	1	*4.145E-005*	*0.73*	*0.4201*	
Residual	3.956E-004	7	5.652E-005			

R^2= 0.7202, Adj R^2=0.8061, Pred R^2=0.8456, Adeq Adeq Precision=26.19

A2. ANOVA. for response surface quadratic model for the flowrate of oxygen as a function of temperature and flowrate of air

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob < F	
Model	1.73	5	0.35	158.69	< 0.0001	significant
A-AIRINLET	1.22	1	1.22	*557.60*	*< 0.0001*	
B-temp	*5.512E-005*	1	*5.512E-005*	*0.025*	*0.8783*	
AB	*9.025E-005*	1	*9.025E-005*	*0.041*	*0.8447*	
A^2	0.63	1	0.63	*288.71*	*< 0.0001*	
B^2	*1.350E-003*	1	*1.350E-003*	*0.62*	*0.4575*	
Residual	0.015	7	2.184E-003			

R^2= 0.9913, Adj R^2=0.9850, Pred R^2=0.9468, Adeq Adeq Precision=29.631

A3. ANOVA for response surface quadratic model for the flowrate of water vapor as a function of temperature and flowrate of air

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob < F	
Model	0.036	5	7.258E-003	108.10	< 0.0001	significant
A-AIRINLET	*0.026*	1	*0.026*	*379.82*	*< 0.0001*	
B-temp	*2.774E-006*	1	*2.774E-006*	*0.041*	*0.8447*	
AB	*2.987E-005*	1	*2.987E-005*	*0.044*	*0.5262*	
A^2	*0.011*	1	*0.011*	*162.50*	*< 0.0001*	
B^2	*3.275E-005*	1	*3275E-005*	*0.49*	*0.5074*	
Residual	4.700E-004	7	6.714E-005			

R^2= 0.9872, Adj R^2=0.9781, Pred R^2=0.7204, Adeq Adeq Precision=25.318

A4. Values of flowrates of nitrogen, oxygen and water vapor against flowrates of air.

Flowrate air (kg/h)	Flowrate of Nitrogen (kg/h)	Flowrate of Oxygen (kg/h)	Flowrate of water-vapor (kg/h)
50	38.499	0.98008	1.3400012
100	76.99	0.06250248	0.01665252
150	115.5	0.09375336	0.002497878
200	153.99	0.06250046	0.033305076

A5. Unit wise specification of process parameters and reactions of PSA UNIT

Unit	Aspen Process Code	Parameters	Value
Air	Stream	Temperature	25⁰C
		Pressure	0.07 N/m²
		Total flow	50 kg/h
		Composition Mass fraction	
		N_2	0.77
		O_2	0.2
		H_2O	0.03
J-T valve	Valve	Pressure	1 Bar
		Temperature estimation	25 K
Compressor	Compressor	Compressor model	Polytropic using GPSA method
		Outlet discharge pressure	5 Bar
Cooler	Cooler	Temperature	25⁰C
		Pressure	0.07 kg/cm²
Splitter	Splitter	Stream 5	
		Stream 6	
		Flash Option	
		Pressure	0.07 kg/cm²
		Valid phase	Vapor-Liquid
Absorber 1	Column RadFrac	Number of stages	33
		Condenser	Total
		Reboiler	Kettle
		Valid phases	Vapor –Liquid
		Convergence	Standard
		Distillate	5.88 E-07 kmol/sec
		Reflux Ratio	0.75 mole

Absorber 2	Column RadFrac	Number of stages Condenser Reboiler Valid phases Convergence Distillate Reflux Ratio	33 Total Kettle Vapor –Liquid Standard 5.88 E-07 kmol/sec 0.75 mole
Mixer 1	Mixer	Pressure Valid phases	0.07 kg/cm^2 Vapor-Liquid
Mixer 2	Mixer	Pressure Valid phases	0.07 kg/cm^2 Vapor-Liquid

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