IOSR Journal of Applied Chemistry (IOSR-JAC)
e-ISSN: 2278-5736.Volume 10, Issue 9 Ver. II (September. 2017), PP 45-60
www.iosrjournals.org

Simulation, Sensitivity Analysis and Introducing New Valid Process Cases in Air Separation Units

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Abstract : *Air separation units are known as one of the most important units in many industries. The purpose of these units is to supply purified Nitrogen and Oxygen to the various parts of the industries for the relevant processes. Hence, obtaining the desired purity of Nitrogen and Oxygen is the key factor of these units' performance. Due to some restrictions of existing technologies, the operating cost and energy consumption of these units are considerably high. In this paper, a comprehensive simulation of the entire industrial cryogenic separation of Nitrogen from the Air will initially be carried out. After that some of the factors affecting the separation in the cryogenic distillation tower such as temperature and pressure of the inlet stream, number of trays and the reflux flowrate will be introduced and examined as sensitivity analysis cases on three different process cases (case A as the design case at 10.21 bar and two new process cases named case B and case C at 5.1 and 20.1 bar, respectively) which has not been published in open literature with this method, in order to illustrate the importance of these factors in designing stage of these units. Two-phase diagram and ternary diagram related to the varied conditions of the inlet stream are implemented to ensure there would not be any azeotrope point in the two-phase region.*

Keywords: *Process simulation, Sensitivity analysis, Nitrogen separation from the Air, Cryogenic process, Cryogenic distillation tower.*

Date of Submission: 08-09-2017 Date of acceptance: 20-09-2017

I. Introduction

The Air in the atmosphere consists mainly of Nitrogen and Oxygen. Elements such as Neon, Argon, Xenon, Krypton and Helium are also presented in very small amounts. Because Air is a rich and free source of Oxygen and Nitrogen, it is used to produce pure gases for industrial purposes. The boiling points of Oxygen and Nitrogen at 1 atmosphere are -182 °C and -196 ° C, respectively. Due to the difference in the boiling points of the air components, these can be separated by a distillation process. The compositions and boiling points of the air is given in the table 1 [1]:

Table 1- Air components

Component	Boiling point (˚C) at 1 atm	Concentration
Nitrogen Oxide	-88	0.35 ppm
Xenon	-108	0.1 ppm
Krypton	-153	1 ppm
Oxygen	-183	20.9%
Argon	-186	0.93%
Nitrogen	-196	78.1%
Neon	-246	18 ppm
Hydrogen	-253	0.5 ppm
Helium	-269	5 ppm

Inlet pressure and the related boiling points are the main factors influencing the Nitrogen separation. Therefore, it is possible to separate Nitrogen from the air stream by reducing its temperature to the desired boiling point. On the other hand, there are different processes and strategies for separating the components in the air, which are rooted in the study of the chemical and physical properties of the air and the costs as will be discussed. Due to the importance of air separation processes, numerous articles have been published to simulate and analyze Air separation units from different aspects. Zheng Jieyu et al. [2] implemented heat pump technique on a single column Air separation unit and showed 39.1% energy saving compared to double column units considering a small variation in maximum pressure from 18 to 20 bar and without taking reflux flowrate into account which may be cost effective. Mehrpooya and Jalali [3] studied air separation unit at 13 bar and -194 °C and used the economic parameters such as interest rate and plant life time for sensitivity analysis instead of operating variables. Pengcheng Ye et al. [4] used membranes to separate Nitrogen from the Air at low feed pressure and temperature down to 100 mbar and -205.25 °C which showed higher selectivity in separation however it is unable to produce high purity Nitrogen.

In previous articles, pressure deviations for sensitivity analysis are limited to the process cases represented by technology owner because of the design pressure limits. In this article the aim is to achieve a comprehensive simulation for the design case (case A), and also two new process cases considering large deviation in inlet temperature and pressure will be presented based on the investigations on two-phase and ternary diagrams to consider azeotrope points in the separation process. In all the presented process cases, a detailed sensitivity analysis will be implemented according to the most effective parameters related to this process, such as number of trays, reflux flow rate and distillate temperature, to investigate the whole plant not only in an extensive inlet condition range but also to change other effective parameters to see whether it is possible to achieve the same purity in other process cases or not.

1.1. Air separation Processes

Nowadays different technologies for air separation are being used, which include cryogenic distillation or refrigeration distillation, membrane separation, pressure swing adsorption and vacuum pressure swing adsorption processes in order to produce high purity Nitrogen streams and the most commonly used process is refrigeration distillation which is operational in various processes of oil, gas and petrochemical industries. In this method, a cold box consists of plate fin heat exchangers, cryogenic distillation tower and expanders are being used for refrigeration with the use of the advantage of the dew points and boiling points to separate the components from the air [5] [6]. Table 2 shows the different methods of air separation and their advantages or disadvantages [1] [7] [8].

Table 2- Different technologies of Air separation

Process	Advantages	Disadvantages
Cryogenic	- Low energy consumption per unit nitrogen -Producing high purity Nitrogen -Ability to produce liquid Nitrogen for storage on the site	- Large scale utility and space required on the site - High capital cost - production capacity limitations - Long time start up or shutdown
Pressure Swing Adsorption	- Low to average capital investment cost - Affordable Nitrogen production with relatively high purity - Easy Installation and start up	-Large maintenance equipment - Noisy operation - production capacity limitations
Membrane	- Low capital cost - Flexible product output - Easy Installation and start up -Easy to change the purity and flow rate	- Uneconomic for very high purity outputs - Uneconomic for large capacity - High energy consumption per unit nitrogen

In this paper the simulation and sensitivity analysis of important parameters of the cryogenic air separation unit has been carried out. The reason for the simulation of this unit is primarily to study the equipment in a process that achieves the temperature and pressure gradients of the equipment which is realized as an important step in the design process. Secondly the purpose of the simulation is to achieve a reliable simulation to make changes to the parameters affecting each equipment and to examine the changes on the equipment in different conditions, and finally to find different operational conditions or process cases that may cause the unit working more efficiently. Among the parameters that influence the separation, it is possible to mention the inlet pressure and temperature of the main stream to the tower, the reflux ratio and the number of trays in the tower, which should be studied to analyze the effects of these parameters on the Nitrogen purity in distillate stream [9]. In order to simulate, Aspen Plus 8.6 software, was implemented. The reasons for using this software are the robustness and accuracy of the calculations of this software to simulate the process, using this software in many scientific papers and the reliability of its calculations.

II. Cryogenic Distillation Process Simulation

In order to simulate cryogenic distillation process, a broad study on the process must be initiated. These studies include the choice of software, a reliable data bank of properties and the equation of state for this process, considering the components in the process and the range of temperature and pressure. The widespread use of the Peng-Robinson equation for simulating air separation units led to simulate this process with respect to this equation of state. The reason for choosing this equation is its ability to predict thermodynamic parameters and properties at low temperatures and in a wide range of pressures [10]. There are very few equation of states that can calculate the molecular interactions and thermodynamic calculations at cryogenic temperatures (about -200 °C) and in the range of near-vacuum pressures up to pressures higher than 100 bar, among which the Peng-Robinson equation of state has been more successful. Consequently, this equation is used in air separation units, gas condensate, refrigeration cycles and low temperature turbines under vacuum and processes containing various hydrocarbons [11]. The Peng-Robinson equation is in fact a correction of the equation of state of the Soave-Ridlich-Kwong, which was presented in 1976 and obtained a significant success in predicting the correct thermodynamic values. In the denominator, this equation of state uses a term different from the previous state equations. The Ping-Robinson equation is written bellow [12].

$$P = \frac{RT}{V_m - b} - \frac{a\alpha}{V_m(V_m + b) + b(V_m - b)}$$

)0-1(

The parameters a, b and α, are defined as:

$$a = 0.45724\,\frac{R^2 (T_C)^2}{P_C}$$

)0-2(

$$\alpha = \left[1 + (1 - T_r^{0.5})(0.37464 + 1.54226\omega - 0.26992\omega^2)\right]^2$$

)0-3(

$$b = 0.07780\,\frac{RT_C}{P_C}$$

)0-4(

$$T_r = \frac{T}{T_C}$$

)0-5(

The Peng-Robinson equation is the most useful state equation for research and industrial purposes, which is widely used to calculate the properties of pure compounds and multiple substances in liquid-vapor and liquid-liquid equilibrium at high and low pressures [12].

2.1. Process Description of Nitrogen Separation from the Air

In this section, the process of producing Nitrogen in the Ilam petrochemical company will be described, which is carried out by cryogenic separation in a cold box. The main stream is the intake air which has a pressure and temperature of 0.86 bar and 20˚C respectively. These values are due to the geolocation of the Ilam Petrochemical Company. Air Intake flowrate is 13562.4 kg/hr. As it is shown in figure 1, The Air is compressed by five compressors to the pressure of 10.5 bar which is the proper pressure for the separation in the designed process to create the two-phase zone for the separation of Nitrogen at -165 °C. Because of the presence of dust and particulates in the air, a filter has been used before entering the air into the compressor. Due to the risk of any probable shut down of the process because of failure of a single compressor, five parallel compressors are considered. Before each one of the compressors, there is an electric heater that performs the task of bringing the unit's inlet stream temperature to 29.85 °C at a constant pressure, so that the compressors are in constant inlet conditions and the unit will be safe at any probable fluctuation of the inlet Air temperature. During the compression process, the Air temperature rises sharply. Therefore, in the compressor output, a heat exchanger shall be used to reduce the flow temperature to the required temperature of the process. These heat exchangers typically use cold water to reduce the compressed air flow temperature to 39.85˚C. The five outlet streams of the compressors are connected together and will eventually enter to a further cooling stage.

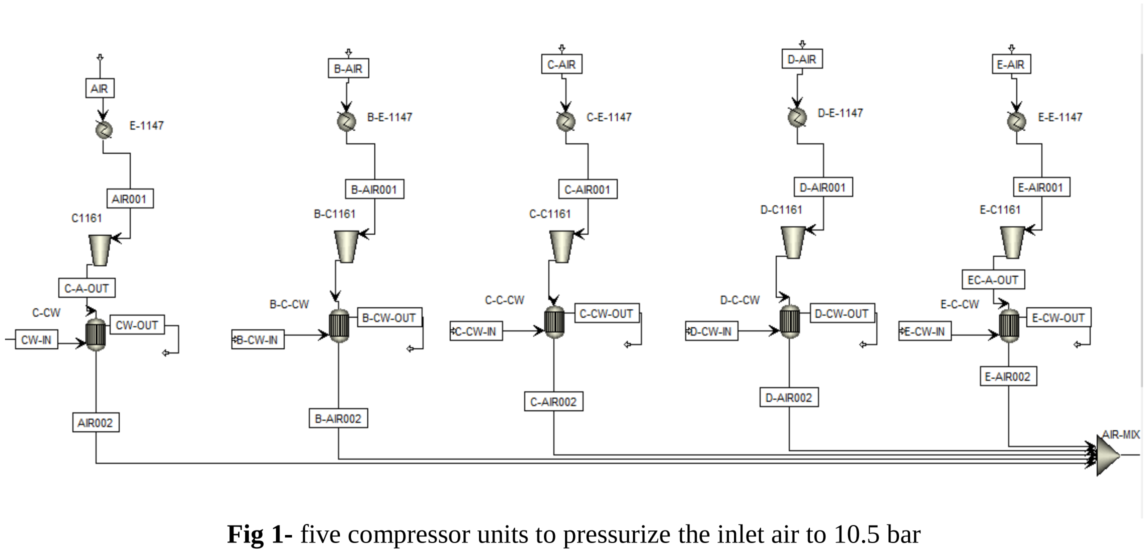


Fig 1- five compressor units to pressurize the inlet air to 10.5 bar

At this stage, the Air stream enters into a cooling tower, which will reduce the air temperature to 18.26 °C, by direct contact with the cooling water as it is shown in figure 2. Some water droplets may be remained in the vapor phase. Because of the implementation of the cryogenic technology, leaving water droplets will lead to freezing the water droplets in the pores of plate fin heat exchangers in the cold box and, consequently, volumetric expansion in those areas that according to the relevant standards of these equipment, ALPEMA, cracking and Even explosion of these exchangers in the cold box are highly possible. So the adsorption towers shall be considered to absorb these water droplets.

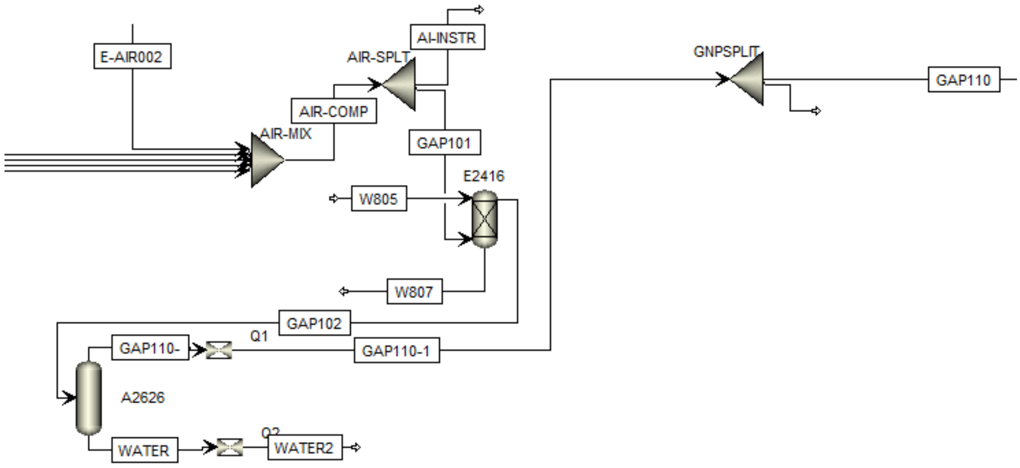


Fig 2- Cooling tower and Adsorption units

After this stage, the stream enters the cold box and the separation of Nitrogen from the air takes place from here onwards, which is shown in figure 3 and 4. The cold box includes a cryogenic distillation tower, a 5 stream plate fin heat exchanger, an expansion turbine associated with control valves and a drums and the related internal piping.

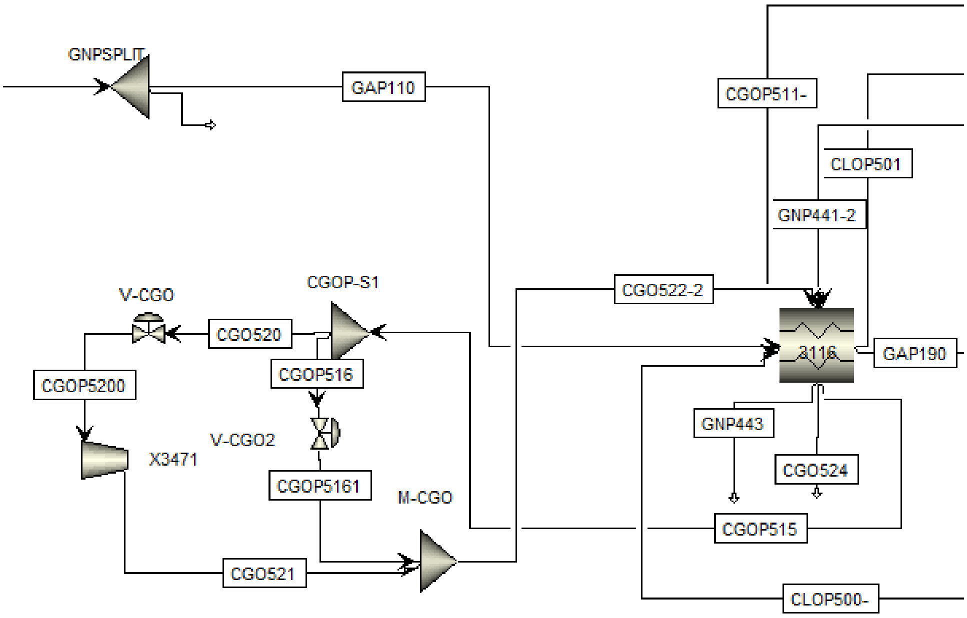


Fig 3- Plate fin heat exchanger and expansion turbine simulation

The Air stream passes through the multi-stream exchanger and its temperature reduced to -165 °C (bubble point of the air in 10.5 bar) and then it is being fed to the bottom of the distillation tower as the main stream. The distillation tower has 60 trays. This tower does not have any reboiler. In order to create a vapor flux from the bottom to the top of the tower, the main flow of the feed to the tower with the vapor phase is used at the bubble point.

The volatile component of the stream, Nitrogen, is purified and extracted from the top of the tower, but the stream at the bottom of the tower will contain a mixture of Nitrogen and Oxygen because the purpose of the unit is to supply a specific purified Nitrogen volume and not any purified Oxygen stream. The type of condenser is a submerged condenser with one inlet stream enters into the shell and two outlet streams from it. A portion of the outlet stream from the condenser, after cooling, is introduced as the reflux stream to the top of the tower to provide required liquid flux for the top of the tower, and the rest enters a drum.

The inlet stream to the expansion turbine is actually a portion of the outlet bottom stream of the tower, which passes through the multi stream heat exchanger then introduces to the shell side of the condenser and then passes through the plate fin heat exchanger again and then enters the expansion turbine as vapor phase. The expansion turbine has the task of expanding the fluid and reducing its pressure and temperature to introduce this stream another time to the multi stream heat exchanger to provide a coolant for the cryogenic separation process.

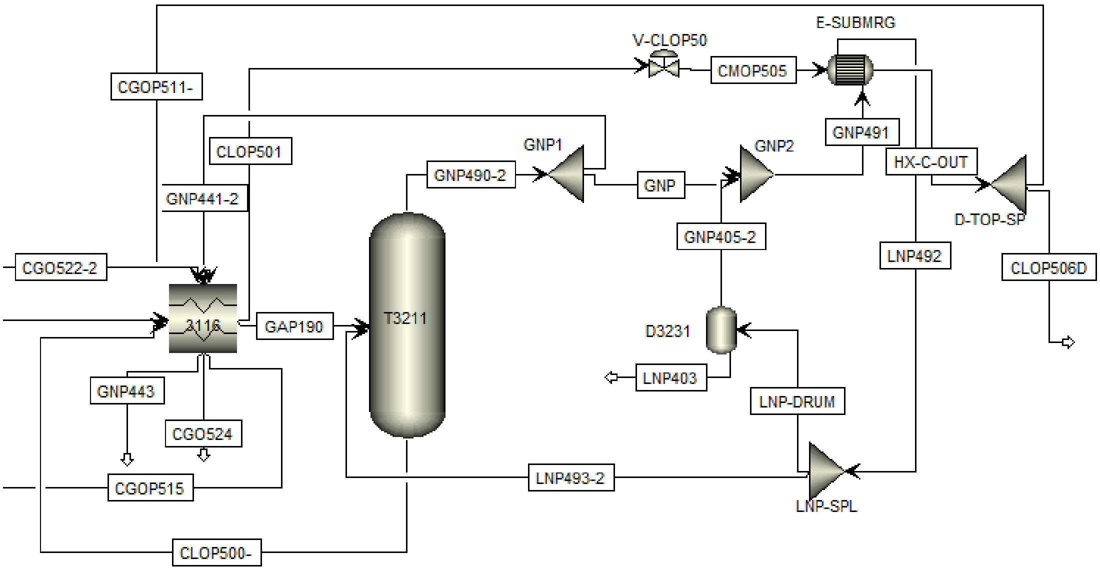


Fig 4- Plate fin heat exchanger, Distillation tower and condenser simulation

III. Results And Discussion

In this section the simulation results if the cold box will be presented.

3.1. Multi stream Heat exchanger (E-3116)

The multi stream heat exchanger (E-3116) has two hot streams (Gap110 and Clop500) and three cold streams (GNP441, CGOP511 and CGO522). The following tables (table 3 to 5) are showing simulated results and the industrial data which are mentioned in the PFD of Ilam Petrochemical company located in Iran.

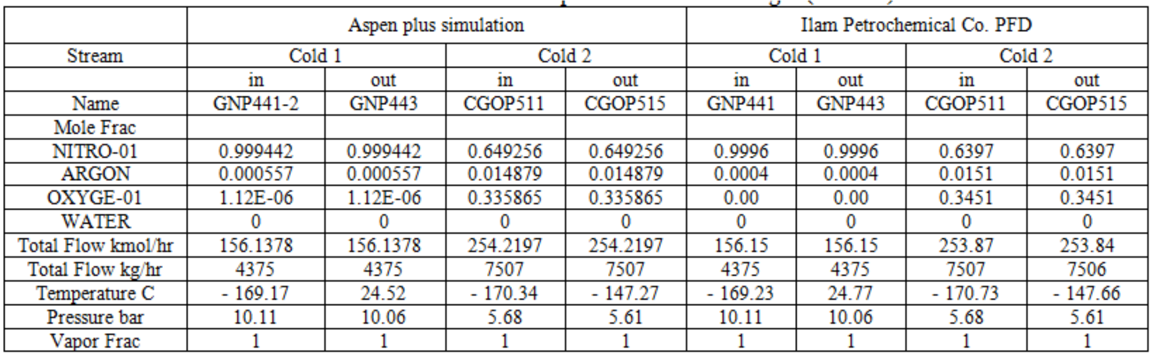
Table 3- Industrial data and Simulation results of plate fin heat exchanger (E-3116) hot streams

	Aspen plus simulation				Ilam Petrochemical Co. PFD			
Stream	Hot 1		Hot 2		Hot 1		Hot 2	
	in	out	in	out	in	out	in	out
Name	GAP110	GAP190	CLOP500	CLOP501	GAP110	GAP190	CLOP500	CLOP501
NITRO-01	0.787	0.787	0.649256	0.649256	0.7812	0.7812	0.6393	0.6393
ARGON	0.009245	0.009245	0.014879	0.014879	0.93	0.0093	0.0151	0.0151
OXYGE-01	0.203755	0.203755	0.335865	0.335865	0.2095	0.2095	0.3455	0.3455
WATER	2.18E-29	2.18E-29	0	0	---	---	---	---
Total Flow kmol/hr	419.7216	419.7216	254.626	254.626	419.38	419.38	254.27	254.27
Total Flow kg/hr	12145	12145	7519	7519	12145	12145	7519	7519
Temperature C	26.85	- 164.92	- 165.02	- 168.55	26.85	- 164.82	- 164.98	- 168.53
Pressure bar	10.27	10.21	10.21	10.21	10.27	10.21	10.21	10.21
Vapor Frac	1	0.998	0	0	1	1	0	0

The main inlet stream to the cold box is Gap110, which passes through the multi stream heat exchanger and enters to the cryogenic distillation tower as the main feed (Gap190). Consequently, the convergence of the Gap190 to the industrial values is the key to the robust and accurate simulation of this unit. The output temperature of the stream, Gap190, in the simulation is -164.92 ° C at 10.21 bar and in industrial documents is -

164.82 ° C at the same pressure, which indicates the accurate simulation of this unit, because this stream shall be as an unknown variable in the simulation. The results of cold streams of this exchanger are as the following tables (tables 4 and 5):

Table 4- Industrial data and Simulation results of plate fin heat exchanger (E-3116) cold streams 1 & 2



	Aspen plus simulation				Ilam Petrochemical Co. PFD			
Stream	Cold 1		Cold 2		Cold 1		Cold 2	
	in	out	in	out	in	out	in	out
Name	GNP441-2	GNP443	CGOP511	CGOP515	GNP441	GNP443	CGOP511	CGOP515
Mole Frac								
NITRO-01	0.999442	0.999442	0.649256	0.649256	0.9996	0.9996	0.6397	0.6397
ARGON	0.000557	0.000557	0.014879	0.014879	0.0004	0.0004	0.0151	0.0151
OXYGE-01	1.12E-06	1.12E-06	0.335865	0.335865	0.00	0.00	0.3451	0.3451
WATER	0	0	0	0	0	0	0	0
Total Flow kmol/hr	156.1378	156.1378	254.2197	254.2197	156.15	156.15	253.87	253.84
Total Flow kg/hr	4375	4375	7507	7507	4375	4375	7507	7506
Temperature C	- 169.17	24.52	- 170.34	- 147.27	- 169.23	24.77	- 170.73	- 147.66
Pressure bar	10.11	10.06	5.68	5.61	10.11	10.06	5.68	5.61
Vapor Frac	1	1	1	1	1	1	1	1

Table 5- Industrial data and Simulation results of plate fin heat exchanger (E-3116) cold stream 3

	Aspen plus simulation		Ilam Petrochemical co.	
Stream	Cold 3		Cold 3	
	in	out	in	out
Name	CGO522-2	CGO524	CGO522-2	CGO524
NITRO-01	0.649256	0.649256	0.6397	0.6397
ARGON	0.014879	0.014879	0.0151	0.0151
OXYGE-01	0.335865	0.335865	0.3451	0.3451
WATER	0	0	0	0
Total Flow kmol/hr	254.2197	254.2197	253.87	253.87
Total Flow kg/hr	7507	7507	7507	7507
Temperature C	-168.90	26.82	-171.19	24.7
Pressure bar	1.18	1.06	1.18	1.06
Vapor Frac	1	1	1	1

Table 6 shows the heat loads of this heat exchanger's streams. According to PFD data, the heat load of this exchanger is 729 kW which has a negligible error in comparison with the simulated value of 720.29 kW.

Table 6- Stream heat loads in Plate fin heat exchanger

Inlet streams	GNP441-2	CLOP500-	CGOP511-	CGO522-2	GAP110
Exchanger side:	COLD	HOT	COLD	COLD	HOT
Outlet stream:	GNP443	CLOP501	CGOP515	CGO524	GAP190
Duty:	263.6399	- 16.6129	52.80853	403.8416	- 703.677

3.2. Cryogenic distillation tower (T-3211):

The streams related to the tower includes the feed stream (Gap190), the distillated stream (Gnp490), the bottom of the tower's outlet (Clop500) and the reflux stream (LNP493). The Simulated and industrial values are shown in table 7.

Table 7- Industrial data and Simulation results of distillation tower (T-3211)

	Aspen plus simulation				Ilam Petrochemical Co. PFD			
Stream	Cold		Cold		Cold		Cold	
	in	out	in	out	in	out	in	out
Name	LNP493-2	GAP190	CLOP500-	GNP490-2	LNP493	GAP190	Clop500	GNP490
NITRO-01	0.999442	0.787003	0.64926	0.999442	0.9996	0.7812	0.6393	0.9996
ARGON	0.000557	0.009245	0.014879	0.000557	0.0004	0.0093	0.0151	0.0004
OXYGE-01	1.12E-06	0.203752	0.335861	1.12E-06	0	0.2095	0.3455	0
WATER	0	2.16E-29	0	0	0	0	0	0
Total Flow kmol/hr	290.1486	419.7218	254.6262	455.2442	290.18	419.38	254.27	455.29
Total Flow kg/hr	8130	12145	7519	12756	8130	12145	7519	12756
Temperature C	- 169.17	- 164.92	- 165.02	- 169.173	- 169.23	- 164.82	- 164.98	- 169.23
Pressure bar	10.11	10.21	10.21	10.11	10.11	10.21	10.21	10.11
Vapor Frac	0	0.998	0	1	0	1	0	1

As it can be seen in the table 7, the purity of the Nitrogen in the distillate stream in PFD is reported 0.9996 which equals with grade 3 of Nitrogen and this value in the simulation is 0.999442, which has a negligible deviation. Also the temperature gradients of the tower converged to the values specified in the industrial papers. In the Ilam Petrochemical Company PFD, the low and high temperatures of the tower are -169.23 °C and -164.98 °C, and in the simulation these values are converged to -169.17 °C and -165.02 °C, respectively. One of the most useful results to analyze the output results of a tower is the purity of each component on each tray which can be used in the form of charts or graphs to study the concentration gradient of components based on their fraction in liquid and vapor phase simultaneously as can be seen in the figure 5:

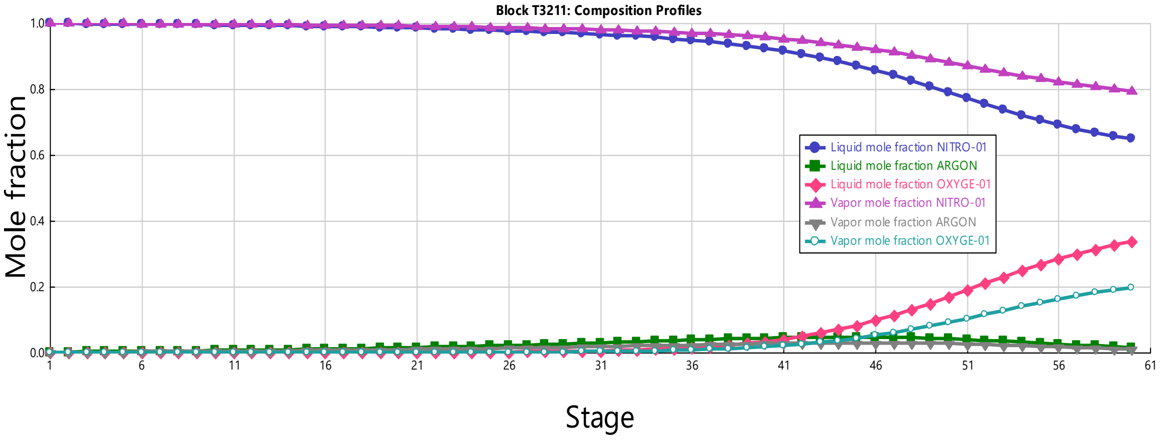


Fig 5- Components mole fractions vs number of trays in the distillation tower

Figure 5 shows that the mole fraction values of volatile components in the vapor phase are higher than the liquid phase on each tray. On the other hand, the mole fractions of the components in the liquid phase for the heavier components is higher than those in the gas phase on each tray, which is due to the unwillingness of that components to evaporate at that stage of separation. The figures 6 and 7 indicate the temperature and pressure gradient of each tray in the tower.

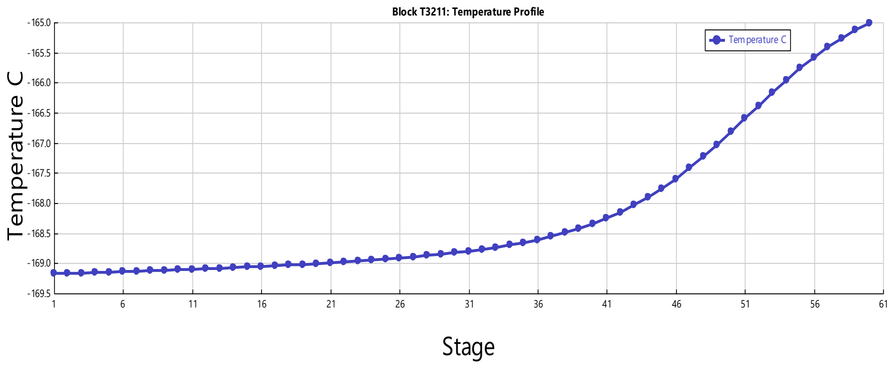


Fig 6- Temperature gradient in distillation tower

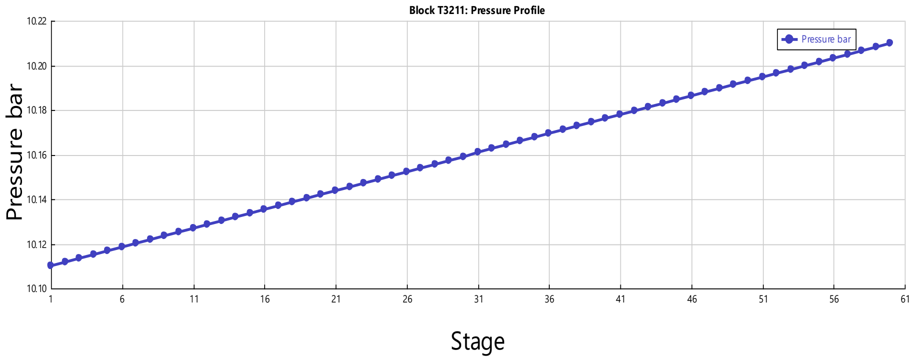


Fig 7- Pressure gradient in distillation tower

3.3. Submerged overhead Condenser (E-3216):

The main hot stream of this condenser is Gnp491, which enters the tube side of the exchanger, and the cold stream is called Cmop505 which enters the shell side. The simulated values and industrial data are mentioned in table 8.

Table 8- Industrial data and Simulation results of Submerged condenser (E-3216)

	Aspen plus simulation				Ilam Petrochemical Co. PFD			
Stream	Inlet		Outlet		Inlet		Outlet	
	Hot	Cold	Hot	Cold	Hot	Cold	Hot	Cold
Name	GNP491	CMOP505	LNP492	HX-C-OUT	GNP 491	CMOP 505	LNP 492	Clop506D+Cgop511
NITRO-01	0.999442	0.64926	0.999442	0.64926	0.9996	0.6393	0.9996	0.6393
ARGON	0.000557	0.014879	0.000557	0.014879	0.0004	0.0151	0.0004	0.0151
OXYGE-01	1.12E-06	0.335861	1.12E-06	0.335861	0	0.3455	0	0.3455
WATER	0	0	0	0	0	0	0	0
Total Flow kmol/hr	299.1064	254.6262	299.1064	254.6262	299.14	254.29	299.14	254.29
Total Flow kg/hr	8381	7519	8381	7519	81381	7519	8381	7519
Temperature C	- 169.17	- 173.71	- 169.18	- 170.34	- 169.23	- 173.73	- 169.23	- 170.73
Pressure bar	10.11	5.68	10.11	5.68	10.11	5.68	10.11	5.68
Vapor Frac	1	0.065	0	1	1	0.06	0	1

3.4. Expansion Turbine X-3471:

In the expansion turbine (X-3471), the high pressure stream (CGO520) enters and the low pressure output stream (CGO521) is being expanded and its temperature will drop as it is shown in table 9.

Table 9- Industrial data and Simulation results of expansion turbine (X-3471)

	Aspen plus simulation		Ilam Petrochemical co.	
Stream	Inlet	Outlet	Inlet	Outlet
Name	CGOP5200	CGO521	CGO520	CGO521
NITRO-01	0.64926	0.64926	0.6397	0.6397
ARGON	0.014879	0.014879	0.0151	0.0151
OXYGE-01	0.335861	0.335861	0.3451	0.3451
WATER	0	0	0	0
Total Flow kmol/hr	138.065	138.065	137.86	137.86
Total Flow kg/hr	4077	4077	4076	4076
Temperature C	- 147.28	- 182.55	-147.66	- 186.15
Pressure bar	5.61	1.18	5.61	1.18
Vapor Frac	1	1	1	1

The purpose of the expansion turbine is to reduce the pressure of the stream which is accompanied by the reduction of temperature. In fact, with an expansion turbine, a stream can be introduced several times at lower temperatures to the multi stream heat exchanger. In the simulation, the pressure drop has been fully performed and the temperature has dropped to -182.55 °C in the simulation and the difference with industrial data was 3.6 ° C which was reported -186.15 °C, but it didn’t have any significant effect on any other stream in the multi stream heat exchanger.

3.5. Changing the effective parameters:

In this section, several effective parameters will be changed and the results will be discussed. Some of the most important parameters affecting the process of Nitrogen separation from Air are the inlet temperature and pressure of the main stream, the number of trays and the reflux flowrate to the distillation tower [13]. Thus three process cases are considered to analyze these parameters from all aspects which are the design case as case A, inlet pressure of 5.1 and 20.1 bar as cases B and C respectively, considering their corresponding temperatures to create a two-phase region which will be discussed.

3.5.1. Case A (Design case):

Separation by distillation towers is based on boiling points difference and volatilities of components. Along the tower, the thermodynamic conditions required for separation must be provided, which are the conditions of temperature and pressure to ensure the existence of a two-phase region [11] [14]. To study the variations in temperature, pressure and the two-phase current range, we can use a two-phase diagram and envelope diagram which are shown in figures 8 and 10.

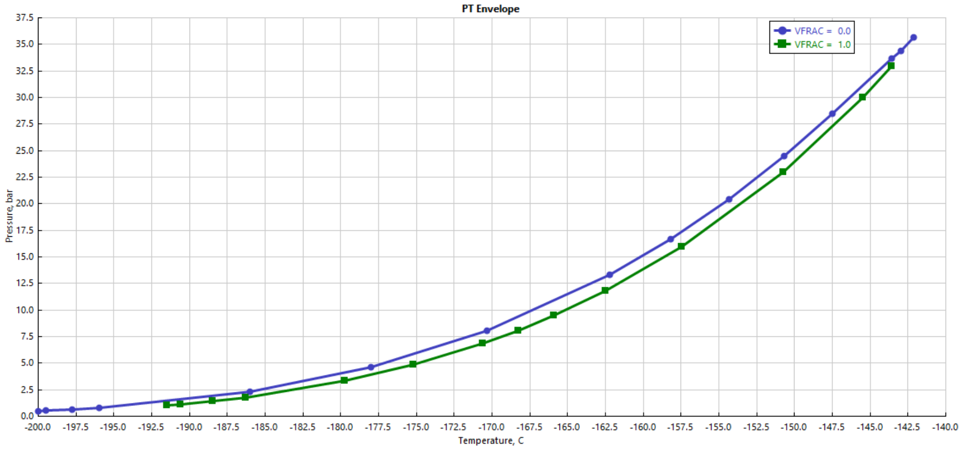


Fig 8- Two-phase diagram for the tower's inlet stream

As shown in the figure 8, the upper and lower curves are obtained by connecting the bubble points and dew points at different temperatures and pressures, respectively. The range between the bubble and dew points is a two-phase region which is suitable for the separation process in the distillation tower [7]. Unlike other streams, this stream does not have a wide-spread two-phase region. Therefore, at a certain gradient pressure, we do not see much temperature variation. According to the industrial data, the temperature changes only 4˚C over 60 trays which shows that this unit shall be designed, operated and controlled precisely to prevent the trays from drying [15]. The design case is based on the pressure and temperature of 10.21 bar and -164.8˚C respectively, which is simulated. The magnified two phase diagram for the design case is shown in figure 9.

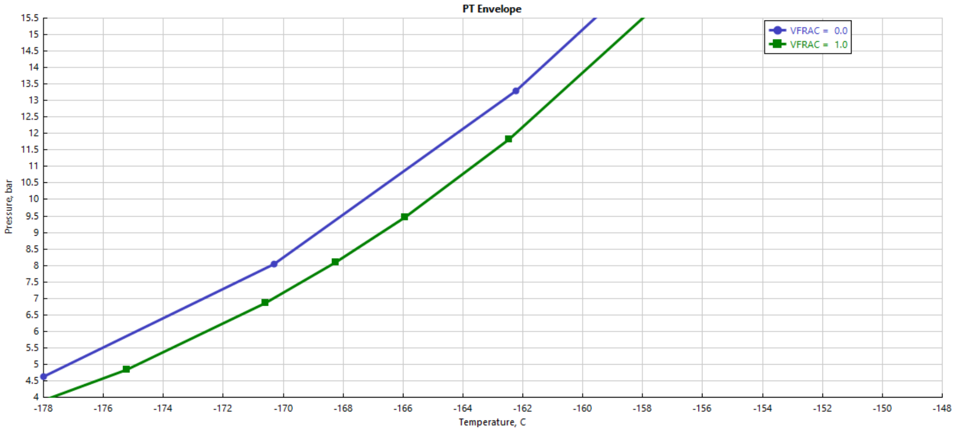


Fig 9- Two-phase diagram for case A (design case) at 10.21 bar

The purpose of this work is merely the sensitivity analysis by changing the conditions, and to show that design pressure is not necessarily the only operational case for the existing unit. The two-phase diagram specifies the existence of the separation region, and the completion of the analysis of this diagram is the use of a ternary diagram depicted on a triangle. Each one of the main three components on each of the three vertices are pure components, and each point inside the triangle expresses the purity of the composition of the mixture of these three components, which is relative to the distance from that point to the vertices of the triangle. In the ternary diagram, the curves are called residue curves that indicate changes in the composition of the liquid phase that evaporates during the separation process in the liquid-vapor equilibrium. The residue curves start from the composition of the feed and continue to the purified or azeotrope points at higher temperatures and pressure conditions [16]. The Separation will not be completed if there are any azeotrope points, in which all the residue lines enters to that knot inside the tringle. Therefore, the analysis of this diagram is required for these units. In the figure 10, a ternary diagram is presented for the feed stream at 10.21 bar.

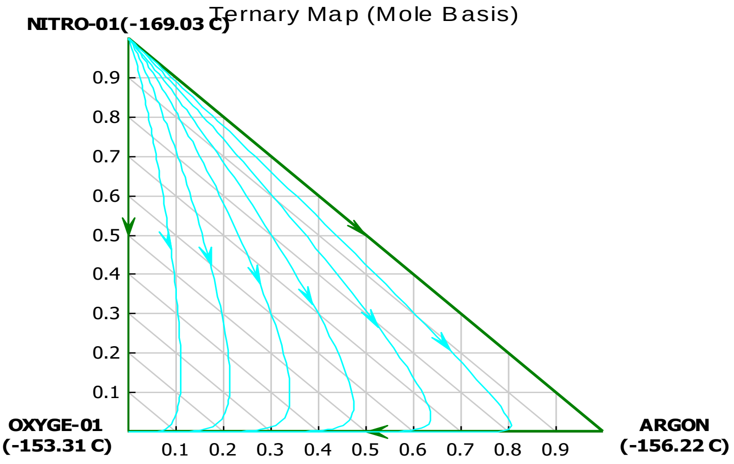


Fig 10- Ternary diagram for case A (design case) at 10.21 bar

The residue curves have not converged to a point other than the vertices of the triangle, therefore there is no azeotrope point at this pressure and temperature range so that the separation by distillation tower in this operating conditions will be possible [17]. In addition, the other variables in the design case are kept constant and the effect of changing the number of trays in the tower (from 10 to 100) is investigated which is mentioned in table 10.

Table 10- The relation of number of trays with Nitrogen purity in case A (design case) at 10.21 bar

Number of trays	Distillate temperature (˚C)	Nitrogen purity in distillate stream
10	-168.71	0.976747
20	-169.063	0.99372
30	-169.144	0.997717
40	-169.162	0.998741
50	-169.169	0.999171
60	-169.173	0.999442
70	-169.176	0.999632
80	-169.178	0.999765
90	-169.179	0.999854
100	-169.180	0.999912

As the number of trays increases, the Nitrogen purity in the distillate stream increases. Increasing the number of trays is very important for purity, because considering 10 trays for the distillation tower, the Nitrogen purity is reported 0.976747 which is not useful for the related process, while with 50 or 60 trays it is possible to achieve Nitrogen grade 3, but for producing grade 4 of Nitrogen the number of trays exceeded to 100 trays which might be impractical and uneconomical in this process condition. The purpose of this unit is to produce grade 3 Nitrogen. In the figure 11, changes in the Nitrogen purity are shown in terms of the number of trays.

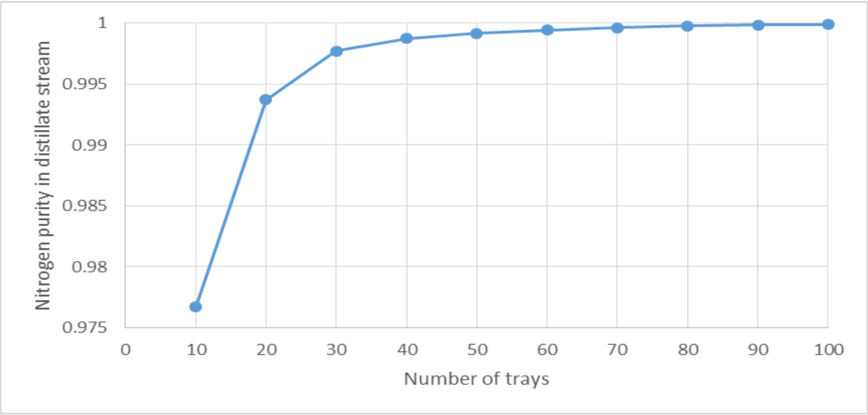


Fig 11- Nitrogen purity vs number of trays in case A at 10.21 bar

In the table 11, the changes in the reflux flow rate and its effect on the Nitrogen purity in the distillate stream above the tower has been investigated.

According to table 11, to obtain products with a purity equivalent to Grade 3, the reflux flowrate should not be less than 8130 kg/hr. In the sensitivity analysis, the number of trays of the tower is considered to be 60 trays. It can be seen that in order to obtain Nitrogen grade 4, the flowrate of the reflux stream shall be increased to 8500 kg/hr. Increasing the reflux flow rate causes to increase the condenser's heat load and operating costs. Figure 12 represents the reflux flow rate changes in term of Nitrogen purity at 10.21 bar.

Table 11- The relation of reflux flowrate with Nitrogen purity in case A at 10.21 bar

Reflux flowrate kg/hr	Distillate temperature (˚C)	Nitrogen purity in distillate stream
6200	-167.213	0.901722
7200	-168.131	0.947727
7700	-168.734	0.977235
8000	-169.132	0.996604
8130	-169.173	0.999442
8500	-169.181	0.99998

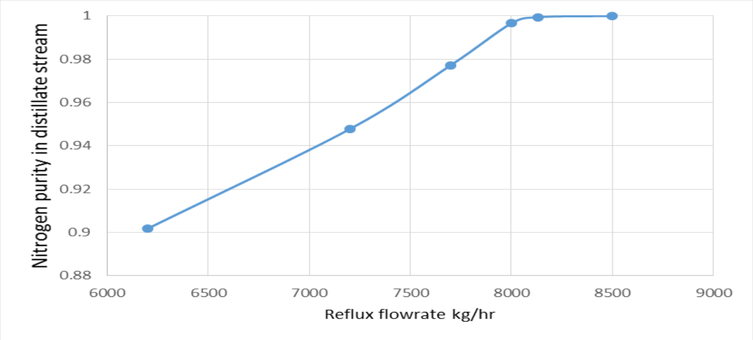


Fig 12- Nitrogen purity vs reflux flowrate in case A at 10.21 bar

3.5.2. Case B (lower inlet conditions):

In this section, the pressure of inlet stream to the distillation tower is changed to a lower value rather than the initial design pressure, which is 5.1 bar and half the design pressure. The two-phase region is practical for the process of separation as can be seen in figure 13.

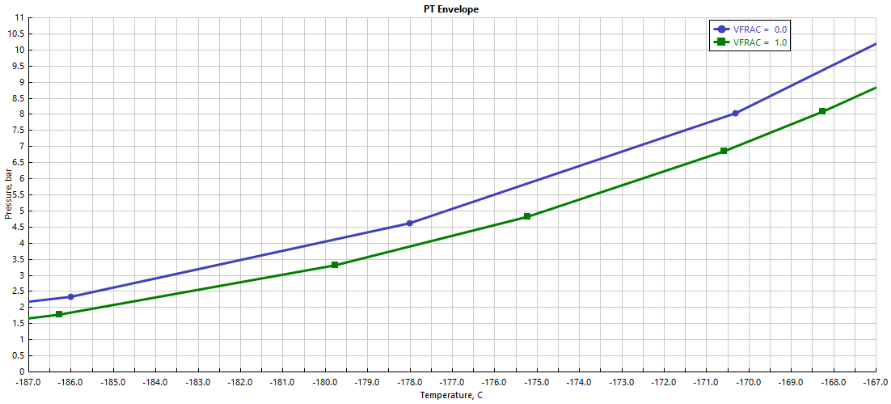


Fig 13- Two-phase diagram for case B at 5.1 bar

According to the two-phase diagram, the corresponding temperature for the separation at 5.1 bar is about -175 °C which is lower than the design case. Considering ternary diagram at 5.1 bar, there is no azeotrope point in figure 14.

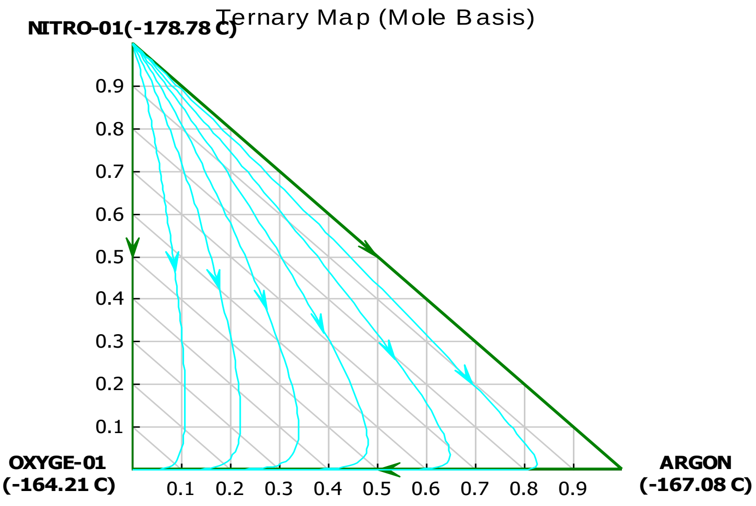


Fig 14- Ternary diagram for case B at 5.1 bar

In the Case B number of trays is changed from 10 to 60, which indicates that with the case B process conditions, with only 20 trays it is possible to achieve the desired grade 3 of Nitrogen purity, and if 60 trays are being used the purity of Nitrogen in distillate stream will reach to much higher grades. Therefore, the lower the pressure of the two-phase region, the lower the temperature of the stream. Table 12 and figure 15 show the relation of the number of trays and the purity of Nitrogen in the distillate stream in case B process conditions.

Table 12- The relation of number of trays with Nitrogen purity in case B at 5.1 bar

Number of trays	Distillate temperature (˚C)	Nitrogen purity in distillate stream
10	-178.937	0.9952632
20	-179.028	0.9997821
30	-179.031	0.9999768
40	-179.032	0.999997
50	-179.032	0.999999
60	-179.032	0.999999

The table 13 and figure 16 indicate the fluctuations of the reflux stream to the tower in relation with Nitrogen purity which show that in order to obtain Nitrogen with grade 3, the flow rate of the reflux stream to the tower can be reduced from 7300 kg/hr which results in the condenser load reduction.

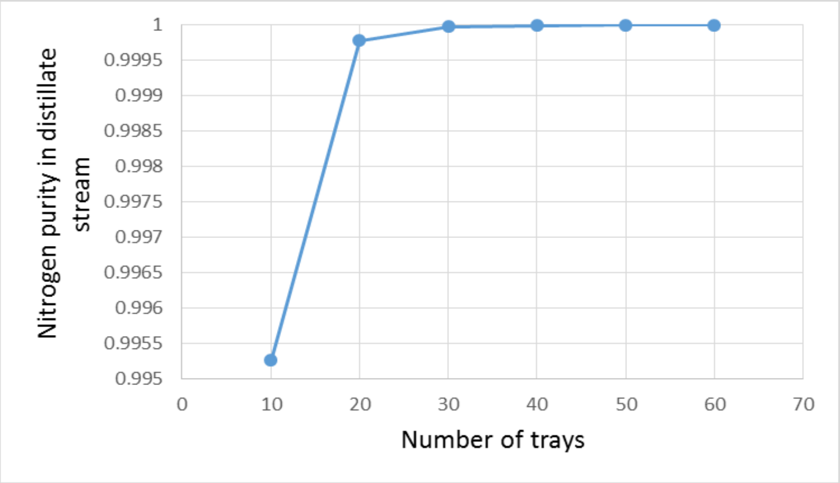


Fig 15- Nitrogen purity vs number of trays in case B at 5.1 bar

Table 13- The relation of reflux flowrate with Nitrogen purity in case B at 5.1 bar

Reflux flowrate kg/hr	Distillate temperature (˚C)	Nitrogen purity in distillate stream
8130	-179.032	0.999999
7505	-179.032	0.999995
7400	179.031	0.999966
7300	-179.03	0.999848
7200	-179.011	0.998539
7100	-178.974	0.995886
7000	-178.839	0.989547

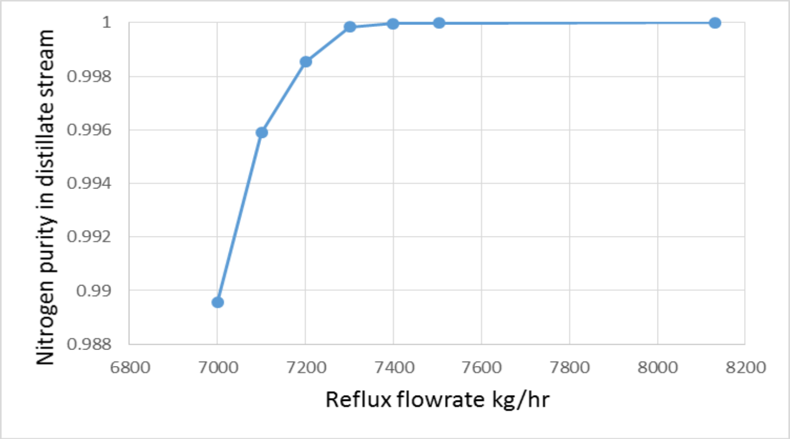


Figure 16- Nitrogen purity vs reflux flowrate in case B at 5.1 bar

3.5.3. Case C (higher inlet conditions):

In case C, the pressure of the inlet stream to the distillation tower is set at a higher pressure than the initial design pressure, which equals with 20.1 bar and is nearly twice the initial design pressure. The two-phase region temperature has increased to -153 °C accordingly. Figure 17 and 18 indicate the possibility of separation in two phase and ternary diagrams.

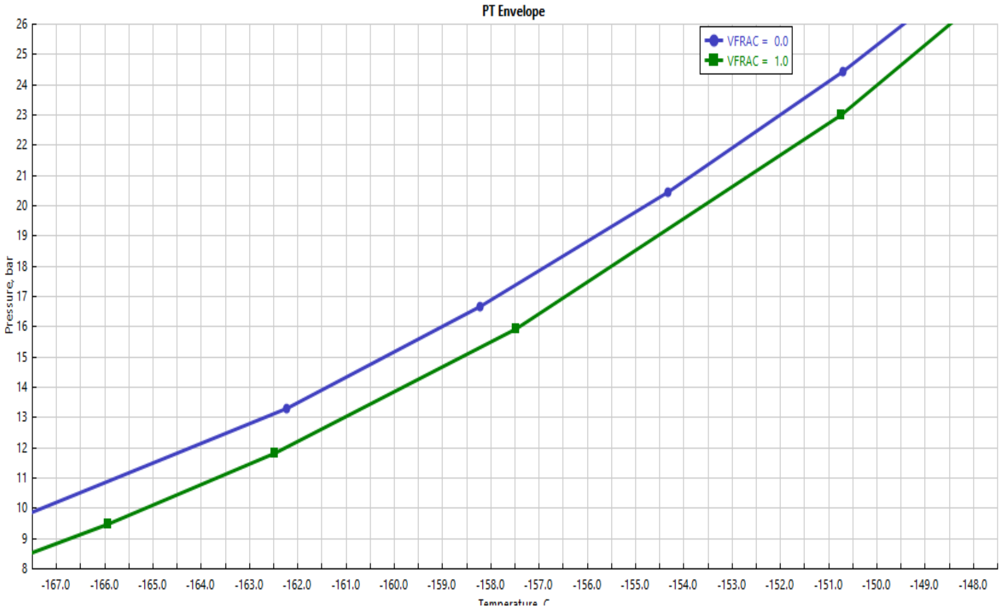


Figure 17- Two-phase diagram for case C at 20.1 bar

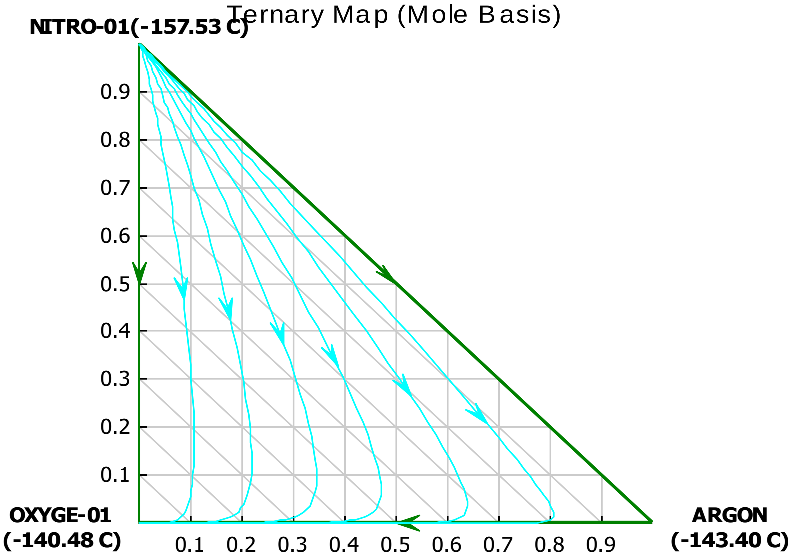


Figure 18-- Ternary diagram for case C at 20.1 bar

The results in case C illustrate that with 60 trays, the purity of Nitrogen is reduced to 93.33209 and it is impractical to achieve higher purity and better separation of Nitrogen. As before, the number of trays in the tower is changed to examine the outlet Nitrogen purity which is shown in table 14 and figure 19.

Table 14- The relation of number of trays with Nitrogen purity in case C at 20.1 bar

Number of trays	Distillate temperature (˚C)	Nitrogen purity in distillate stream
5	-155.688	0.900983
10	-156.129	0.92356
20	-156.302	0.93239
40	-156.319	0.933208
60	-156.319	0.933209
100	-156.319	0.93321

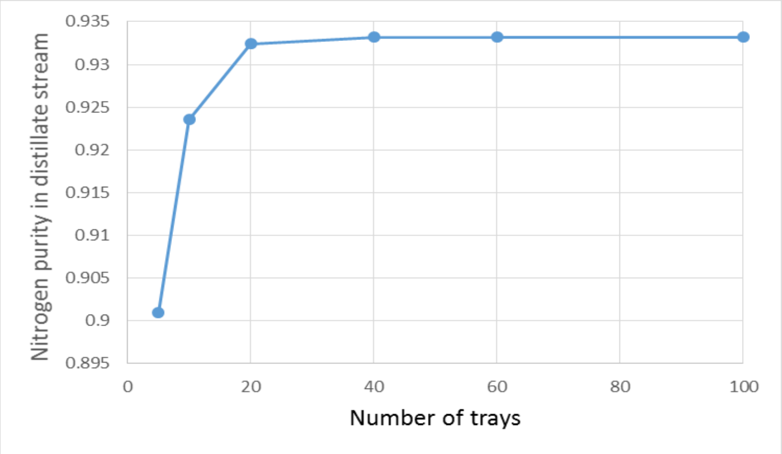


Fig 19- Nitrogen purity vs number of trays in case C at 20.1 bar

Also table 15 and 20 show the variation of Nitrogen purity related to the reflux flowrate which result that with reflux flowrate of 8130 kg/hr, Nitrogen separation with 93.3% of purity can be achieved at 20.1 bar, and this value will not be increased even if the number of trays would be increased, but it would still be possible to improve Nitrogen purity to grade 3 with increasing reflux flowrate up to 9500 kg/hr which results in higher condenser loads.

Table 15- The relation of reflux flowrate with Nitrogen purity in case C at 20.1 bar

Reflux flowrate kg/hr	Distillate temperature (˚C)	Nitrogen purity in distillate stream
7130	-155.482	0.890247
8130	-156.319	0.933208
8500	-156.728	0.954024
8800	-157.115	0.97363
9200	-157.588	0.998003
9500	-157.615	0.999782
9800	-157.618	0.999965

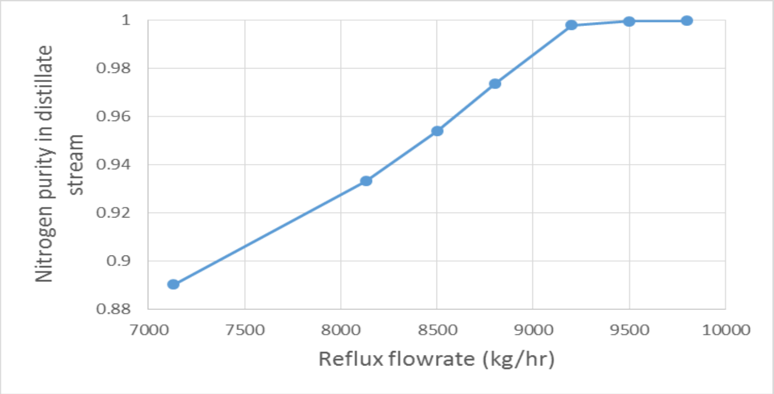


Fig 20-- Nitrogen purity vs reflux flowrate in case C at 20.1 bar

IV. Conclusion

In this study, a comprehensive simulation for the air separation unit of Ilam Petrochemical Company has been carried out to separate Nitrogen from Oxygen which can be used to study the concentration gradient of different components in the cryogenic distillation tower, as well as the temperature gradient along it. All equipment in this unit are simulated and converged to industrial quantities with a negligible error of less than 1%. After obtaining a reliable simulation model, some changes were made to the effective parameters. Several parameters such as the temperature and pressure of the inlet stream into the distillation tower, number of trays in the distillation tower and the reflux flowrate were investigated, which were changed in different process cases with initial pressures of 10.21 bar (as case A or design case), 5.1 and 20.1 bar as new cases named B and C respectively.

In order to analyze the changes, two-phase and ternary diagrams were considered and the residue curves were plotted in the ternary diagram to ensure that there is no azeotrope point in the two-phase region. Then the input pressure was changed from 10.21 bar to 5.1 and 20.1 bar to determine its effect on separation. On the other hand, in the design case and two new process cases, the number of trays in the tower were changed from 10 to 100 trays and it was observed that by increasing the number of trays the separation would be operated better and the purity of Nitrogen can be increased up to grade 5 or 6. However, this variable is directly related to the reflux flowrate. Therefore, the change in reflux flowrate was investigated to examine its effect on the Nitrogen purity for the three process cases and the appropriate ranges for obtaining Nitrogen with the desired purity in the new cases were found.

The result of the changing the reflux flowrate is that the purity of the final product is directly related to the reflux flowrate, but the condenser load will be increased in higher flowrates simultaneously. Finally, the diagrams of changing the number of trays and the reflux flowrate were plotted in terms of the purity of Nitrogen in the distillate stream which showed a significant rise in purity of Nitrogen by increasing the related values.

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Mehran Moazeni Targhi. “Simulation, Sensitivity Analysis and Introducing New Valid Process Cases in Air Separation Units .” IOSR Journal of Applied Chemistry (IOSR-JAC), vol. 10, no. 9, 2017, pp. 45–60.