

Modeling And Optimization For Nitrogen Liquefaction With Subcooling And Air Separation Unit From Air

Animesh Saini, Surajit Ghosh, Sayan Kar, Pranta Sutradhar, Sourav Poddar

Abstract: Nitrogen liquefaction is an energy-intensive process which is used in several industries like polymer industry, aerospace engineering, air separation unit, sewage treatment plant, electronic industry, agricultural science, petroleum and reservoir engineering, mining engineering, bioscience engineering, nanotechnology, separation process technology, storage technology, civil and construction engineering, fuel cell, catalysis, power systems, pharmaceutical technology, ceramic technology, solar energy systems, molecular dynamic simulation etc. Also, nitrogen can be utilized for the manufacture of ammonia or start tipping on an ammonia plant, protection of materials from bacterial and fungal disorders. Therefore, liquefaction of nitrogen is an important process for various process industries. Generally, liquefaction of nitrogen involves various methods like reverse stirling cycle, LINDE-HAMPSON cycle, Joule Thompson effect and etc. This research is focused on the production of generation of liquid nitrogen from air using Air Separation Unit (ASU) followed by multistage subcooling system. Modeling of this process was carried out using Aspen Plus® and then optimized using Design Expert®. The final composition of liquid nitrogen varies from 78.558 tons/day to 234.7108 tons/day, which increases linearly, while the conversion of 78.558% to 78.224%, which decreases exponentially. The effect of parameters used in the Design Expert ® were split fraction (f) and air flowrate (a). The values of (f) and (a) were fixed using User Defined Method, Central Composite Method and D-Optimal Method. User Defined Method confirms that when the air flowrate was 299.99 tons/day with a split fraction of nitrogen from ASU unit is 0.59, the production of liquid nitrogen is 132.1815 tons/day. While for Central Composite Method and D-optimal Method, when the air flowrates were 300 and 299.99 with split fraction of 0.6 and 0.59 respectively then the production of liquid nitrogen were 128.8224 and 139.975 respectively. Out of these three response methodology methods D-Optimal Methods reveals the most appropriate method since it infers the maximum nitrogen production or generation. The range for the production or generation of liquid nitrogen validates with the results of Aspen Plus ®. So it can be confirmed that the results obtained from Aspen Plus ® are realistic in nature.

Index Terms: Aspen Plus®, liquid nitrogen, multistage system, optimization, Air Separation Unit (ASU)

I. INTRODUCTION

Air mainly comprises of nitrogen, oxygen, water vapor and some traces of dusts and other particles and particulate matters and other gases, shown in the Appendix A.3. Amongst all nitrogen is the major component. Nitrogen is an inert compound and can be utilized by various industries as a cryogenic compound.[1,7,44,45] Cryogenic and non-cryogenic systems are used for air separation to recover nitrogen gas that are further liquefied to utilise in many industrial sectors like polymer[1,2,4, 17], aerospace engineering [3,4], air separation unit [5,6], sewage treatment plant [7], electronic industry [8,9,10], agricultural science [9], petroleum and reservoir engineering [11,12,14], mining engineering [12,13], bioscience engineering [15], nanotechnology [15], separation process technology [15], storage technology [16], civil and construction engineering [17], fuel cell [18], catalysis [18], power systems [18], pharmaceutical technology [19], ceramic technology [20], solar energy systems [20], molecular dynamic simulation [21]. Podbielniak [22] first proposed the use of refrigerant for cryogenic refrigeration in 1936. After that USA initiated a program for the development of a \$1000 cryocooler [23]. Recently Praxair has patented several processes for liquefaction of gases and air separation using mixed refrigerant cycles [24-25]. These cycles engage non-flammable mixtures. Air Products has patented mixed refrigerant and turbine processes on liquefaction of nitrogen [26]. Their mixture dwells with nitrogen and hydrocarbon refrigerants. Although cryogenic methods provide high purity products, non-cryogenic methods such as pressure swing absorption (PSA) or membrane separation are much energy-efficient depending on the proper design of the plant and processes. We have focused on modelling of separation of nitrogen from air and liquefying nitrogen considering theoretical smoke and fog effects [7]. We have simulated this process using Aspen Plus® and optimized using Design Expert®. This work presents a process design for liquefaction of nitrogen with subcooling in a multistage refrigeration system, where main component nitrogen (refrigerant) is taken from the PSA unit [29]. Our aim is to calculate the maximum production rate of liquid nitrogen using Aspen Plus® [30-32] and Design Expert® [33]. Though the design calculation does not give the real-life production environment but it can provide relief from making wide range of experiments without making the small-scale reactor plant.

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I. METHODOLOGY

The whole system was calculated using Aspen Plus ® [30-32], which is shown in the figure 1. and then the final flowrates of N₂ was optimized using Design Expert ® [33].

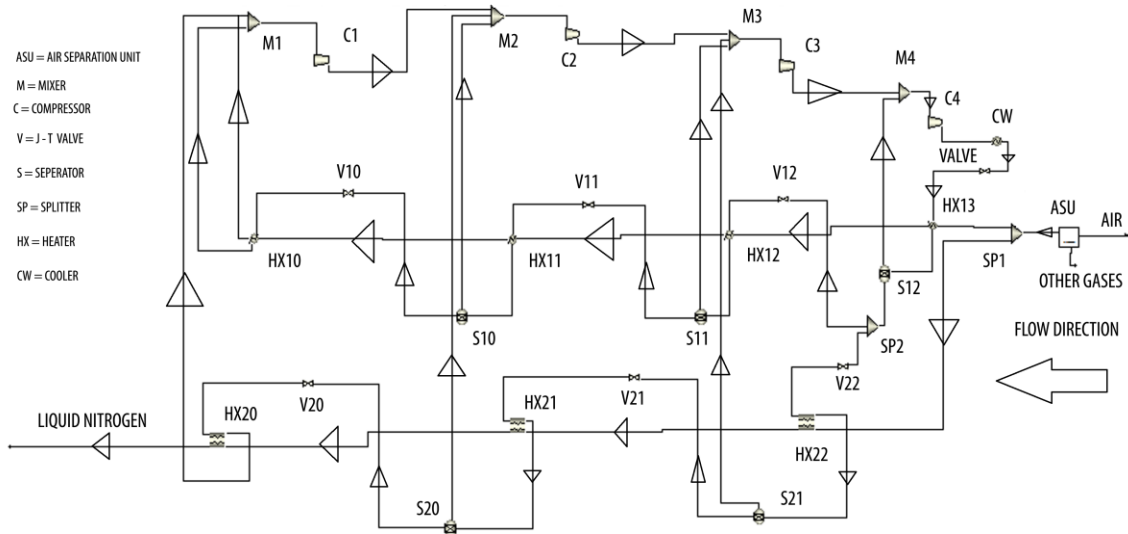


Figure 1: Process block diagram for production of liquid nitrogen from air.

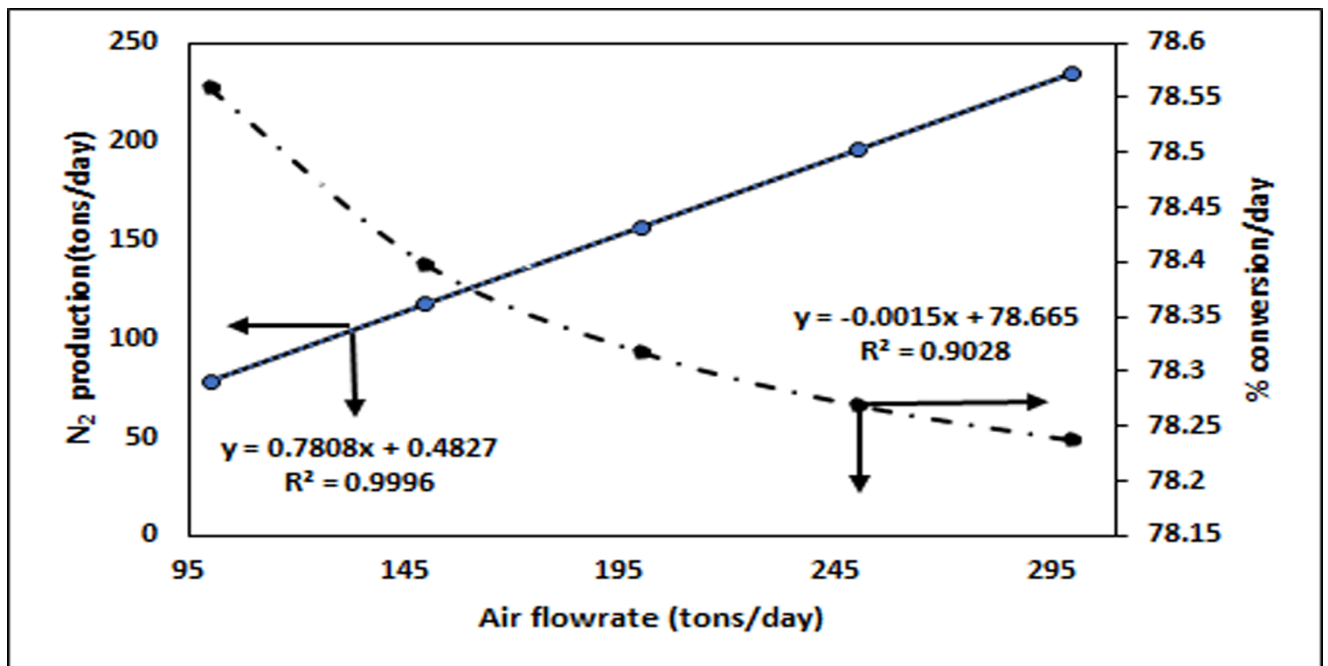


Figure 2: Variation in production of nitrogen production (tons/day) against air flowrates (tons/day)

Table 1: Variation in production of nitrogen (tons/day) against air flowrates (tons/day)

Air Flowrate (tons/day)	Nitrogen Production (tons/day)	% production of liquid Nitrogen (Conversion)
100	78.55877241	78.55877241
150	117.5967958	78.39786387
200	156.6348192	78.3174096
250	195.6728426	78.26913703
300	234.710866	78.23695533

Design-Expert® Software

Nitrogen Production

234.61

78.45

X1 = A: Nitrogen Production

X2 = B: split fraction

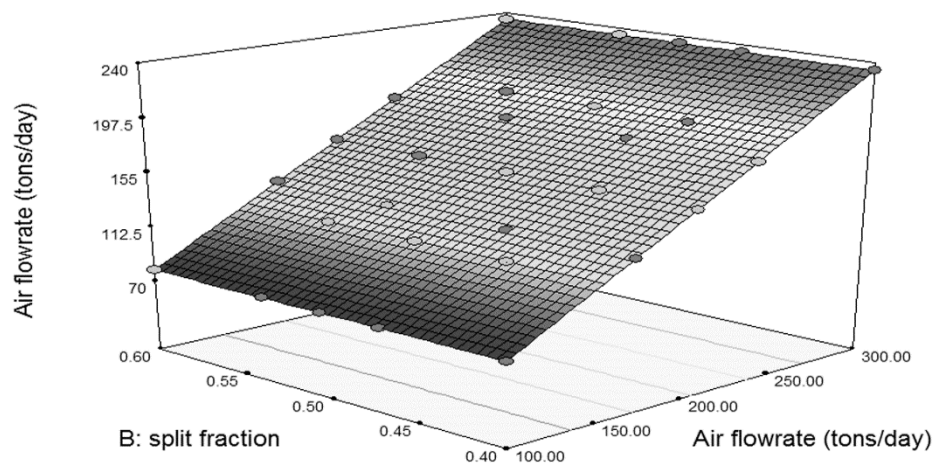


Figure 3: The production of nitrogen as a function of split fraction ratio of nitrogen inlet in HX22 and air flowrate (tons/day) [USER DEFINED METHOD]

Table 2: ANOVA for response surface quadratic model for the production of liquid nitrogen as a function of air flowrate and split fraction ratio of nitrogen inlet in HX22

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F	
Model	75373.36	5	15074.67	2.64E+06	< 0.0001	significant
A-Nitrogen Production	75372.96	1	75372.96	1.32E+07	< 0.0001	
B-split fraction	0.29	1	0.29	50.54	< 0.0001	
AB	7.20E-06	1	7.20E-06	1.26E-03	0.972	
A ²	0.095	1	0.095	16.65	0.0005	
B ²	0.011	1	0.011	1.91	0.18	
Residual	0.13	23	5.71E-03			

$R^2=0.9998$, $Adj R^2=0.9997$, $Pred R^2=0.9995$, $Adeq Precision=339.616$

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Design-Expert® Software

Nitrogen Production
 234.71
 78.45
 X1 = A: Air Flowrate
 X2 = B: split fraction

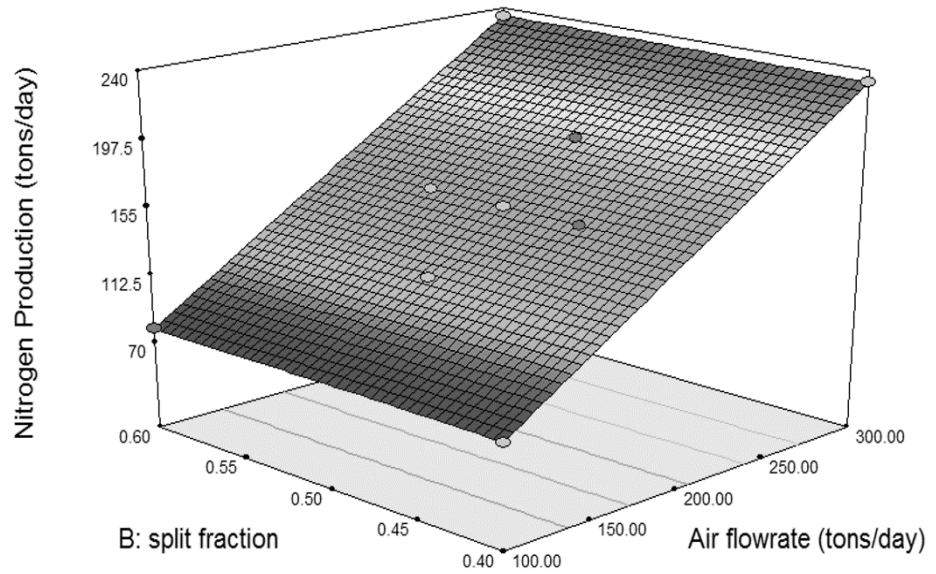


Figure 4: The production of nitrogen as a function of split fraction ratio of nitrogen inlet in HX22 and air flowrate (tons/day) [CENTRAL COMPOSITE METHOD]

Table 3: ANOVA for response surface quadratic model for the production of liquid nitrogen as a function of air flowrate and split fraction ratio of nitrogen inlet in HX22

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F	
<i>Model</i>	26198.25	5	5239.65	2.71E+05	< 0.0001	<i>significant</i>
<i>A-Air Flowrate</i>	26195.8	1	26195.8	1.35E+06	< 0.0001	
<i>B-split fraction</i>	0.94	1	0.94	48.69	0.0002	
<i>AB</i>	0.8	1	0.8	41.42	0.0004	
<i>A²</i>	8.79E-03	1	8.79E-03	0.45	0.5218	
<i>B²</i>	7.08E-03	1	7.08E-03	0.37	0.5643	
<i>Residual</i>	0.14	7	0.019			

$R^2=0.9988$, $Adj R^2=0.9898$, $Pred R^2= 0.9997$, $Adeq Precision= 348.171$

Design-Expert® Software

Nitrogen Production
234.61
78.45
X1 = A: Air flowrate
X2 = B: split fraction

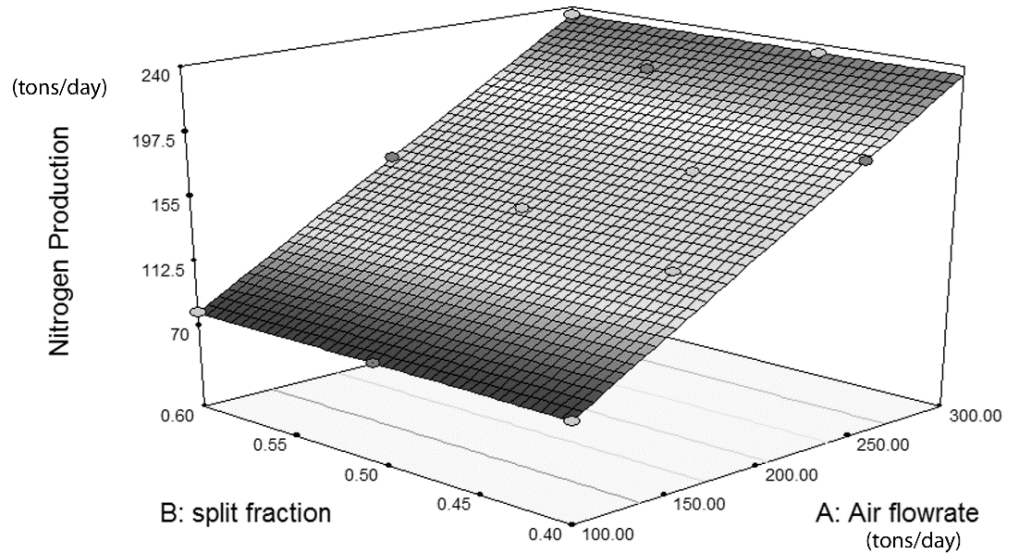


Figure 5: The production of nitrogen as a function of split fraction ratio of nitrogen inlet in HX22 and air flowrate (tons/day) [D-OPTIMAL METHOD]

Table 4: ANOVA for response surface quadratic model for the production of liquid nitrogen as a function of air flowrate and split fraction ratio of nitrogen inlet in HX22

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F	
Model	61657.17	5	12331.43	7.58E+06	< 0.0001	significant
A-Air flowrate	54332.46	1	54332.46	3.34E+07	< 0.0001	
B-split fraction	0.032	1	0.032	19.47	0.0013	
AB	2.89E-05	1	2.89E-05	0.018	0.8966	
A ²	0.11	1	0.11	64.87	< 0.0001	
B ²	9.73E-03	1	9.73E-03	5.98	0.0345	
Residual	0.016	10	1.63E-03			

R² = 0.9999, Adj R² = 0.9997, Pred R² = 0.8625, Adeq Precision = 228.904

2.1. Aspen Plus® Modelling

Aspen Plus® was used for the liquefaction of Nitrogen from atmospheric air [44]. It provides accurate results compared to the real life [26] and comprehensive thermodynamics basis for accurate determination of physical properties [29], transport properties and phase behavior [27]. The present simulation was conducted using ideal and Peng-Robinson models [32,42, 43] which fits best to equilibrium since components are gaseous and non-polar. The components used were N₂ (non-polar) and O₂ (non-polar) and others [44,45]. Figure 1. shows the production of nitrogen from air using ASU followed by liquefaction with subcooling. The whole process simulation was carried out using the following assumptions:

- Process is substantial state and isothermal.
- Air comprises of nitrogen, oxygen, water vapor (H₂O) and other components [7].

- All the components are gases and were used from the Aspen Plus® library itself.
- All the streams lines that were used based on SI units.
- Peng-Robinson models and Ideal models fits the equation of state [EOS].
- All the unit processes were based on SI units.

2.2. Process Description:

For simulation purpose, it was assumed air composed of nitrogen, oxygen, small traces of water vapor and others [44,45]. The detailed composition of air is shown in the table A.3. The detailed procedure of the systems as follows:

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- Initially the simulation was investigated for 100 tons/day with temperature and pressure was set at 298K (25 °C) and 7×10^7 bar. Later the flowrates were varied to 300 tons/day.
- The gas stream (air) enters into Air Separation Unit (ASU) [30], with nitrogen as main stream excluding all other components of air.
- The final outflow from the ASU [30] was split into two parts. One part enters Heat Exchanger (HX22) and the other at Heat Exchanger (HX13). According to the previous researchers, Lee et. al [29], it comprises of five stages, but for simplification we have divided into halves apart from five stages.
- The split fraction was initially set at 0.4, later on it was also varied from 0.4 to 0.60. to obtain the maximum liquid nitrogen production.
- The whole sub-cooling process is divided into two halves. The upper half comprises of four Heat Exchangers (HX13, HX12, HX11 and H10) Mixers (M1, M2, M3 and M4), compressors (C1, C2, C3 and C4), three J-T (Joule Thomson) valves (V12, V11 and V10), four separators (S12, S11, S10 and SP2) and one cooler (CW) and one normal valve. The lower half comprises of three Heat Exchangers (HX22, HX21 and HX20), J-T (Joule Thomson) valves (V21, V22 and V20) and two separators (S21 and S20). The detailed calculation of the Air Separation Unit and sub-cooling process is shown in the Appendix as A1. and A2. respectively.
 - The upper half produces the gaseous nitrogen, whereas lower half produces liquid nitrogen. The gaseous nitrogen is recycled and fed to the MIXER (M1) in to order to maximize the production or generation of liquid nitrogen. The nitrogen produced or generated from the Air Separation Unit (ASU) was having a pressure of 6.87 kPa, which was then compressed to 250, 420 and 750 kPa and finally to 1730 kPa. The compressed gas was then liquefied and subcooled through the cooler (CW) and the liquid pure nitrogen was isentropically expanded through the Joule–Thompson (J–T) valve. Like compression, expansion was also designed in the multiple stages. The pure nitrogen cooled and the mixed gas passages over the stages. In each stage, the vaporized pure refrigerant sent to the compressor and the liquid fraction was expanded to the next stage. Thereafter, the pure nitrogen was sent to the compressor again, and these series of steps were repeated to obtain the maximum production.
- The simulation was based on a plant using 100 [30], 150, 200, 250 and 300 tons/day (TPD) respectively of air using the Air Separation Unit (ASU) [30] and multistage subcooling process [29], in order to obtain the optimized flowrate of nitrogen.
- To rigorously simulate the pure refrigerant process, Aspen plus® modelling was used where the equation of state [EOS] was selected as Peng–Robinson [32,] because it is recommended for pharmaceutical and biotechnology industries [reactor cooling, lyophilization, VOC treatment and recovery], metal production [heat treatment, Inerting], chemical industries [Nitrogen stripping

and recovery, Inerting], aerospace and aircraft [autoclave inerting and heat treatment] [35].

- The minimum temperature differences of each heat exchanger (HX22, HX21, HX20) were 298, 368, and 353 K, in the refrigeration system, in order to attain the temperature of the liquid nitrogen. Therefore, the outlet temperature of the hot stream was set to be 279.15 K. The flow rates of the gaseous nitrogen were determined under the assumption that all gaseous nitrogen was vaporized but not superheated while passing through the final heat exchanger. The convergence method used for the simulation was Newtonian with complex optimization method. The Tear stream convergence parameters were tolerance limit as “0.0001”, trace option as “Cutoff” and state as “Pressure and Enthalpy”. The sequence parameters were design specification nesting as “with tear”, User nesting as “outside”, Variable weight and loop weight as “1” for both the cases. The Solver used for the simulation was “LSSQP (Large Scale Successive Quadratic Programming)”. The detailed Aspen Plus ® coding is shown in the Appendix as A1 and A2 respectively, where A1 represents the unit wise specification of process parameters and reactions of ASU UNIT and A2 represents the unit wise specification for Nitrogen liquefaction with subcooling.

2.3. Parametric Sensitivity and Optimization

The effects of parameters namely: split fraction (f) and air flowrate (a) of air that are two major response variables namely, A and B were correlated mathematically in this work. The model equations were developed with the aid of response surface methodology [36,40,41] varying the values of f and a simultaneously. The values of (f) and (a) were fixed using user defined method, central composite method and D-OPTIMAL method [37,38]. The reason of selecting three methods is to find the best suited method. The mathematical relationships between the responses (Y_i) and factors, air flowrates (X₁) and split fraction (X₂) are given by,

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

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

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

The significance of the coefficients and the adequacy of the fit were determined using Student-t test and Fischer F-test [39, 40] respectively. The values of flowrates of Nitrogen were maximized respectively. The development of model equation and optimization has been done using Design -Expert Software 7.0 ® [33,40,41].



3. Results and discussion

After performing the simulation, it was observed that the production or generation of liquid nitrogen was maximum at 300 tons/day. The final flowrates variation against nitrogen production or generation obtained from Aspen Plus ® are shown in the figure 2. It is clearly evident from figure 2 and table 1 that the flowrates of nitrogen continuously increase as the flowrates of air increases, whereas the conversion decreases as the flowrate of air increases. Therefore, we can confirm that final composition of nitrogen varies from 78.558 tons/day to 234.7108 tons/day, which increases linearly, while the conversion from 78.558% to 78.224%, which decreases exponentially. This clearly indicates that the production of nitrogen increases with the increase in the air flowrate (tons/day) but the conversion decreases with the increase in air flowrate. The ideal condition for the production and conversion of nitrogen would be 130 tons/day and 78.35% when the air flowrate was 160 tons/day.

$$y_i = \alpha_i + \sum_{j=1}^2 \beta_{ij} X_j + \sum_{j=1}^2 \sum_{u=1}^2 \beta_{iuj} X_u X_j + \sum_{j=1}^2 \beta_{ijj} X_j^2 \quad (3)$$

$u \neq j$

$$\begin{aligned} \text{Nitrogen Production} = & -7.23246 \\ & - 7.092E - 003 * \text{air} - \text{flowrate} \\ & + 33.88564 * \text{split} - \text{fraction} \\ & + 0.20936 * \text{air} - \text{flowrate} * \text{split} - \text{fraction} \quad (4) \\ & + 2.0857E - 005 * \text{air} - \text{fraction}^2 \\ & + 36.0318 * \text{split} - \text{fraction}^2 \end{aligned}$$

$$\begin{aligned} \text{Nitrogen Production} = & -4.50914 \\ & - 0.010879 * \text{Air} - \text{flowrate} \\ & + 22.13078 * \text{split} - \text{fraction} \\ & + 0.25067 * \text{Air} - \text{flowrate} * \text{split} - \text{fraction} \quad (5) \\ & + 8.67E - 06 * \text{Air} - \text{flowrate}^2 \\ & - 25.68636 * \text{split} - \text{fraction}^2 \end{aligned}$$

$$\begin{aligned} \text{Nitrogen Production} = & 12579.29076 \\ & + 37.32334 * \text{Air} - \text{flowrate} \\ & - 89995.44606 * \text{split} - \text{fraction} \\ & - 202.51463 * \text{Air} - \text{flowrate} * \text{split} - \text{fraction} \\ & + 0.049646 * \text{Air} - \text{flowrate}^2 \quad (6) \\ & + 2.19E + 05 * \text{split} - \text{fraction}^2 \\ & + 0.18013 * \text{Air} - \text{flowrate}^2 * \text{split} - \text{fraction} \\ & + 157.34967 * \text{Air} - \text{flowrate} * \text{split} - \text{fraction}^2 \\ & - 2.46E - 04 * \text{Air} - \text{flowrate}^3 \\ & - 1.68E + 5 * \text{split} - \text{fraction}^3 \end{aligned}$$

The variation in flowrates of nitrogen obtained by varying the flowrates of air and split fraction of nitrogen from the separation unit (SP2) in order to the optimum condition. The optimum condition was determined using response surface methodology. Design Expert® software was used for this purpose. The quadratic equations, predicted by the statistical modelling can be considered as equation no.3.

Figure 3, 4 and 5 shows the flowrates of nitrogen as a function of split fraction ratio of nitrogen production from ASU unit and air flowrate (tons/day). From the ANOVA table, provided in Table.2,3 and 4 the probability values were less than 0.0001, which makes the model fit for the maximum production of liquid nitrogen. The model equations obtained during modelling of the process is a surface quadratic type, since the significant terms of the equation ends at square terms. The model equation for optimum nitrogen flowrates is shown below as equation no.4, 5 and 6. Hence, from the model equation (4), table 2 and Figure 3, it can be confirmed that when the air flowrate is 299.99 tons/day with a split fraction ratio of nitrogen from ASU unit was 0.59, then the production of nitrogen was 128.8224 tons/day, when USER DEFINED MODEL was used. The model equation (5), table 3 and figure 4 suggests that when the air flowrate is 300 tons/day with a split fraction ratio of nitrogen from ASU unit was 0.6, the production of nitrogen was 132.1815 tons/day, when Central Composite METHOD was used. The model equation (6), table 4 and figure 5 recommends that when the air flowrate was 299.99 tons/day with a split fraction of nitrogen from ASU unit was 0.59, the production of nitrogen was 139.975 tons/day, when D-Optimal Method was used. From the Anova Table, D-Optimal Method suggests that the Adeq Precision was less compared to the other two Methods, i.e. the ratio of the range of variation in the predicted response to an estimate of the standard error of the predictions was less compared to others. The The Predicted R² of 0.8625 was in reasonable agreement with the Adjusted R² of 0.9997. The range for the production or generation of nitrogen using Design Expert® software varied from 128.22 to 139.975 tons/day. This results validates the results the obtained from Aspen Plus ®. So it can be confirmed that the results obtained from Aspen Plus® were realistic with respect to Design Expert® results.

4. Recommendation for future scope (Conclusion)

Demand of liquid nitrogen is increasing from time to time, so in order to meet this demand many industries, especially pharmaceutical, food, air conditioning, nuclear, transportation, shipping and etc. Liquefaction of nitrogen from common source like ambient air with minimal expenditure is alarming. Simple reverse Stirling cycle process is the most common and other basic process of liquefaction of nitrogen from ambient air, but apart that this method will be beneficial to utilize for better performance and efficiency wise, since it shows that the production or generation of liquid nitrogen increases with the variation in air-flowrate and split fraction ratio with a minimal decremental in the efficiency.



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Aspen Plus® was used to design the whole process including the process conditions. The final outcome of the Aspen Plus® Simulator has been represented in the article, where it depicts that the generation or production rate of liquid nitrogen increases with the increase in the flowrate of air but the percentage conversion decreased with the increase in the flowrate of air. The ideal condition for the production and conversion of nitrogen would be 130 tons/day and 78.35% when the air flowrate was 160 tons/day. Then the results of Aspen Plus® were fitted in to the Design Expert® optimizer to observe the optimum conditions. The optimum nitrogen production or generation is 128.8224 tons/day, 132.1815 tons/day and 139.975 tons/day when USER DEFINED, CENTRAL COMPOSITE and D-Optimal Methods were used respectively with the air-flowrate was almost 300 tons/day with a split fraction ratio of nitrogen from ASU unit was 0.6 almost. Out of these three methods D-Optimal Methods reveals the most prominent method, since the production of nitrogen is maximum in the case of D-Optimal method. The F- value for D-Optimal Method is 5972.76, which implies that the model is significant and there is only a 0.0001% chance of error than that of other F-values. The results of Design Expert® validates with the results of Aspen Plus®. Thus proofing the results of Aspen Plus® to be a realistic one in nature. A huge scope lies in the improvement and simulation of this process, as this calculation lacks energy exchange with surroundings. So the advancement in this direction is inevitable. Further advancement lies in the LCA development, technical development and techno-economic feasibility of the process.

Conflicts of interest

There are no conflicts to declare

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Appendix

A1. Unit wise specification of process parameters and reactions of PSA UNIT

Unit	Aspen Process Code	Parameters	Value
Air	Stream	Temperature	25 ^o C
		Pressure	0.07 N/m ²
		Total flow	50 kg/h
		Composition	
		Mass fraction	
		N ₂	78.084
		O ₂	20.046
		Ar	0.9340
		CO ₂	0.04
		Ne	0.001818
He	0.000524		
H ₂ O	0.893658		
Splitter (SP1)	FSplit	Stream1 Stream2	0.4, 0.45, 0.5, 0.55
J-T valve	Valve	Pressure Temperature estimation	1 Bar 25 K
Compressor	Compressor	Compressor model Outlet discharge pressure	Polytropic using GPSA method 5 Bar
Cooler	Cooler	Temperature	25 ^o C 0.07 kg/cm ²
Splitter	Splitter	Pressure	
		Stream 5	
		Stream 6	
		Flash Option	
Absorber 1	Column RadFrac	Pressure	0.07 kg/cm ²
		Valid phase	Vapor-Liquid
		Number of stages	33
Absorber 1	Column RadFrac	Condenser	Total
		Reboiler	Kettle
		Valid phases	Vapor-Liquid
		Convergence	Standard
		Distillate	0.0009488 kmol/sec
		Reflux Ratio	0.85 mole

Absorber 2	Column RadFrac	Number of stages Condenser Reboiler Valid phases Convergence Distillate Reflux Ratio	33 Total Kettle Vapor –Liquid Standard 0.0009488 kmol/sec 0.85 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

A2. Unit wise specification for Nitrogen liquefaction with subcooling

Unit	Aspen Process Code	Parameters	Value
Heater (HX13)	Heater	Temperature	9 °C
		Pressure	21.78 atm
		Valid Phases	vapor-liquid-free-water
Separator (SP2)	SEP	Outlet stream	16 7
		sub stream	MIXED MIXED
		Component ID	N ₂ = 0.5 (OUTLET STREAM = 16)
Splitter	FSplit	Stream 19	0.5
		Stream 15	0.5
		Valve (V22)	VALVE
Heater (HX22)	MHeatX	Flash options Valid phase Maximum iteration Error tolerance	Vapor – liquid 30 0.0001
		Inlet stream	3 14
		Exchanger side	COLD HOT
		Outlet stream	13 12
		Valid Phase Specification	VAPOR ONLY VAPOR-LIQUID
		Temperature Value	5
		Unit	C
		Pressure	29
		Unit	atm
		Duty Estimate Unit	watt watt
Max iterations	90 30		
Tolerance	0.0001 0.0001		
Mixer (M4)	Mixer	Pressure	
		Valid phases	vapor-liquid-free-water
		Temperature estimate	10 °C
		Convergence parameters Maximum iteration Error tolerance	90 0.0001
		Compressor (C4)	Compr
Cooler (CW)	Heater	Efficiencies Isentropic	0.75
		Temperature	200 °C
		Pressure	1 atm
Valve (V12)	VALVE	Valid phases	Vapor-liquid
		Calculation Type Adiabatic flash for specified outlet pressure (pressure change) Pressure specification Outlet pressure	1atm
		Flash options Valid phase Maximum iteration Error tolerance	Vapor – liquid 30 0.0001

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Valve (V21)	VALVE	Calculation Type	
		Adiabatic flash for specified outlet pressure (pressure change)	
		Pressure specification	
		Outlet pressure	1atm
		Flash options	
		Valid phase	Vapor – liquid
		Maximum iteration	30
		Error tolerance	0.0001
HEATER (HX12)	MHeatX	Temperature	8 °C
		Pressure	42.28 atm
		Valid phases	Vapor-liquid-free-water
HEATER (HX21)	MHeatX	Inlet stream	43
		Exchanger side	Cold
		Outlet stream	37
		Valid Phase	Liquid only
		Specification	Temperature
		Value	-100
		Unit	C
		Pressure	
		Unit	N/sqm
		Duty Estimate	
		Unit	Watt
		Max iterations	30
		Tolerance	0.0001
Separator (S11)	SEP	Outlet stream	23
		sub stream	MIXED
		Component ID	N ₂ = 0.5 (OUTLET STREAM = 23)
Valve (V11)	VALVE	Calculation Type	
		Adiabatic flash for specified outlet pressure (pressure change)	
		Pressure specification	
		Outlet pressure	2.5 atm
		Flash options	
		Valid phase	Vapor – liquid
		Maximum iteration	30
		Error tolerance	0.0001
HEATER (HX11)	MHeatX	Temperature	7 °C
		Pressure	62.78 atm
		Valid phases	Vapor-liquid-free-water
Separator (S20)	SEP	Outlet stream	39
		sub stream	MIXED
		Component ID	N ₂ = 0.6, O ₂ =0.5, (OUTLET STREAM = 39)
Mixer (M3)	Mixer	Pressure	6 atm
		Valid phases	vapor-liquid
		Temperature estimate	10°C
		Convergence parameters	
		Maximum iteration	30
		Error tolerance	0.0001
Mixer (M2)	Mixer	Pressure	
		Valid phases	vapor-liquid
		Temperature estimate	-30°C
		Convergence parameters	
		Maximum iteration	30
		Error tolerance	0.0001
Compressor (C3)	Compr	Isentropic	
		Discharge pressure	2.467 atm
		Efficiencies	
		Isentropic	0.75
Compressor (C2)	Compr	Isentropic	
		Discharge pressure	7.402 atm
		Efficiencies	
		Isentropic	0.75

Compressor (C1)	Compr	Isentropic	
		Discharge pressure	17.07 atm
		Efficiencies	
Mixer (M1)	Mixer	Isentropic	0.75
		Pressure	
		Valid phases	vapor-liquid
		Temperature estimate	-70°C
		Convergence parameters	
		Maximum iteration	30
Separator (S10)	SEP	Outlet stream	26 25
		sub stream	MIXED MIXED
		Component ID	N ₂ = 0.6 (OUTLET STREAM = 25)
Valve (V10)	VALVE	Calculation Type	
		Adiabatic flash for specified outlet pressure (pressure change)	
		Pressure specification	
		Outlet pressure	2 atm
		Flash options	
		Valid phase	Vapor – liquid
		Maximum iteration	30
		Error tolerance	0.0001
Valve (V20)	VALVE	Calculation Type	
		Adiabatic flash for specified outlet pressure (pressure change)	
		Pressure specification	
		Outlet pressure	1 atm
		Flash options	
		Valid phase	Vapor – liquid
		Maximum iteration	30
		Error tolerance	0.0001
HEATER (HX10)	MHeatX	Temperature	6 °C
		Pressure	83.28 atm
		Valid phases	Vapor-liquid-free-water
HEATER (HX20)	MHeatX	Inlet stream	45 36
		Exchanger side	Cold Hot
		Outlet stream	40 41
		Valid Phase	Liquid only Liquid only
		Specification	Temperature
		Value	-180
		Unit	C
		Pressure	85
		Unit	N/sqm N/sqm
		Duty Estimate	
		Unit	Watt Watt
		Max iterations	30 30
Tolerance	0.0001 0.0001		

A3. Major constituents of dry air, by volume

Gas	Formula	% (volume percentage)
Nitrogen	N ₂	78.084
Oxygen	O ₂	20.046
Argon	Ar	0.9340
Carbon Dioxide	CO ₂	0.04
Neon	Ne	0.001818
Helium	He	0.000524
Water vapor	H ₂ O	0.893658